# A NEW NUMERICAL APPROACH FOR THE SOLUTION OF CONTAMINANT TRANSPORT EQUATION

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## ABSTRACT

In this paper we show that the Wavelet-Galerkin method is a very effective tool in numerically solving contaminant transport equation. The approach is applied to a number of examples and numerical results are given. The numerical results demonstrate the reliability and efficiency of using the Wavelet-Galerkin method to solve such problems.

**Keywords:** Wavelet-Galerkin method, contaminant transport equation, numerical solutions

## 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 Wavelet-Galerkin method to solve the contaminant transport equation:

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

subject to boundary conditions

$$u(0,t) = 0, \quad u(1,t) = 0, \qquad (2)$$

and the initial conditions

$$u(x,0) = \eta(x), \quad 0 < x < 1, \qquad (3)$$

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 diffusion 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 [8] and Hornung [12].

In recent years, a lot of attention has been devoted to the study of Wavelet-Galerkin method to investigate various scientific models. The efficiency of the method has been formally proved by many researchers (Amaratunga [1], Avudainayagam [2, 3], Beylkin [4], El-Gamel [9], Glowiniski [10], Jaffard [13], Jin [14], Ming-quayer [17, 18], Qian [20, 21], Xu [24]).

The paper is organized as follows. In Section 2 and 3 we give a brief discussion on the wavelets and connection coefficients. The Wavelet-Galerkin solution for equation (1) is described in detail in section 4. In Section 5, we apply our method to specific problems, compare the results, and close with conclusions.

## MULTIRESOLUTION ANALYSIS AND WAVELET BASIS

MRA is an important concept in wavelet theory. Many useful orthonormal wavelets are constructed within its framework. In order to give a good explanation of the relationship between MRA and wavelet basis, we introduce the following definitions (Boggess [5], Daubechies [6, 7], Mallat [15], Walnut [23]).

*Definition* 1. We call a wavelet any function $\psi(t) \in L^2(R)$ satisfying:

$$\int_{-\infty}^{\infty} |\hat{\psi}(w)|^2 |w|^{-1} dw < \infty \qquad (4)$$

Generally, we deal with the wavelets whose Fourier transforms are continuous. In that case, the wavelet $\psi(t)$ must be undulant, i.e.

$$\int_{-\infty}^{\infty} \psi(t) dt = 0 \qquad (5)$$

*Definition 2.* We call a multiresolution analysis (MRA) the sequence of close subspaces $\{V_j\}_{j\in Z}$ such that the following conditions are satisfied:

- $\ldots V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \subset \ldots$
- $f(x) \in V_J \Leftrightarrow f(2x) \in V_{J+1}, \quad J \in Z$
- $\cup_{J\in Z} V_J = L^2(R)$, and $\cap_{J\in Z} V_J = \{0\}$.
- There exists a scaling function $\phi(t) \in V_0$ such that
  $V_0 = \overline{\text{span}\{\phi(t-n), \quad n \in Z\}}$

The significance of MRA lies in its relationship with the orthonormal wavelet basis. It means that an orthonormal wavelet basis can be derived from an MRA, which is a direct result of the following theorem.

Theorem 1. Let $\{V_j\}_{j\in Z}$ be an MRA and $\phi(t)$ its scaling function. Assume that the collection $\{\phi(x-n), n \in Z\}$ forms an orthonormal basis for $V_0$. We write the so-called two-scale difference equation

$$\phi(x) = \sum_{i=0}^{L-1} P_i \phi(2x - i), \qquad (6)$$

$$\psi(x) = \sum_{i=2-L}^{1} (-1)^i P_{1-i} \phi(2x - i), \qquad (7)$$

where the coefficients $P_i (i = 0, 1, \ldots, L-1)$ appearing in the 2-scale relations (6) and (7) are called the wavelet filter coefficients. The support of the scaling function $\phi$ is the interval [0, $L$−1] while that of the corresponding wavelet $\psi$ is the interval [1−$L$/2, $L$/2]. The Daubechies wavelet filter coefficients for L = 4, 6, 8 and 10 are listed in Jin [14].

Writing

$$\psi_{Jk}(x) = 2^{J/2}\psi(2^J x - k), \quad J, k \in Z. \quad (8)$$

We have that the collection of wavelets $\{\psi_{Jk}(x), \quad J, k \in Z\}$ forms a complete orthonormal basis for the space $L^2(R)$.

Actually, Theorem 1 shows how to construct an orthonormal wavelet basis from an MRA. For instance, the orthonormal Daubechies wavelet bases are constructed by means of Theorem 1. It is well known that an orthonormal basis can be easily applied to the signal decomposition and analysis. Hence the MRA method shall be regarded as an important framework of wavelet applications.

We define $V_J$ as the closure of the space generated by $\{\phi_{Jk}(x) = 2^{J/2}\phi(2^J x - k), \quad J \succ 0, k \in Z\}$ and $W_J$, its orthogonal complement in $V_{J+1}$, as the closure of the space generated by $\{\psi_{Jk}, \quad J, k \in Z\}$. This condition implies that

$$V_{J+1} = V_J \oplus W_J \quad (9)$$

where $\oplus$ denotes the orthogonal direct sum. The space $L^2(R)$ is represented as a direct sum

$$L^2(R) = \oplus_{J \in Z} W_J. \quad (10)$$

On each fixed scale $J$, the wavelets $\{\psi_{Jk}(x)\}_{k \in Z}$ form an orthonormal basis of $W_J$ and the scaling functions $\{\phi_{Jk}(x)\}_{k \in Z}$ form an orthonormal basis of $V_J$. The set of spaces $V_J$ is called a multiresolution analysis of $L^2(R)$. These spaces will be used to approximate the solutions of partial differential equations using the Galerkin method.

## CONNECTION COEFFICIENTS

Any numerical scheme for solving differential equations must adequately represent the derivatives of the unknown functions. In the case of wavelets bases, these approximations give rise to certain $L^2$ inner products of the basis functions, their derivatives and their translates, called the connection coefficients. The numerical approximation of the connection coefficients which appear with the wavelet bases is unstable since the integrals are highly oscillatory. To overcome this difficulty, specific algorithms have been devised by (Ming-quayer [17]) for the exact evaluation of the connection coefficients. Since the scaling functions and wavelets do not have explicit analytic expressions but are implicitly determined by the two scale relations (6) and (7), it is necessary to develop algorithms to compute several connection coefficients, which occur in the application of the Wavelet-Galerkin procedure to differential and integral equations.

For solving Equation (1) in the bounded interval [0, 1], we need to calculate the following two connection coefficients:

$$M_k^m(x) = \int_0^x y^m \phi(y-k)dy. \quad (11)$$

$$\Gamma_k^n(x) = \int_0^x \phi^{(n)}(y-k)\phi(y)dy. \quad (12)$$

Algorithms for computing the connection coefficient (11) are given by (Ming-quayer [17]). The computation of the connection coefficient (12) is reported by (Ming-quayer [17]) with the exception that the normalizing conditions are replaced by:

$$\sum_{k=m-L+2}^{m-1} K^n \Gamma_k^n(m) = n!\,\Theta_1(m) - (-1)^n \left[ \sum_{2-L \le k \le m-L+1} K^n \Gamma_{-k}^n(L-1) \right]. \quad (13)$$

where $\Theta_1(x) = \int_0^x \phi(y)dy$ , and its computation is reported (Ming-quayer [17]).

## WAVELET-GALERKIN METHOD

In this section, we will solve the problem given by Equations (1)–(3) by using the Wavelet-Galerkin method. Let the solution $u_J(x,t)$ of the problem be approximated by its $J$-th level wavelet series on the interval (0,1), i.e.,

$$u_J(x,t) = \sum_{k=2-L}^{2^J-1} u_{J,k}(t)\phi_{Jk}(x), \quad \mathrm{k} \in Z, \quad (14)$$

where $\phi_{Jk}(x) = 2^{J/2}\phi(2^J x - k)$, $J > 0$. and $u_{J,k,} k = 2-L, 3-L, \ldots, 2^J-1$ are $2^J+L-2$ unknown coefficients to be determined. Here, the integer $J$ is used to control the smoothness of the solution. The larger integer $J$ is used, the more accurate a solution can be obtained. However, the number of equations required to solve the unknown coefficients is increased. In (14), the parameter $L$ represents that the wavelet associated with the set of $L$ Daubechies filter coefficients is used as the solution bases. Substituting the wavelet series approximation $u_J(x, t)$ in equation (14) for $u(x, t)$ in equation (1), yields:

$$A\frac{d}{dt}u_{J,k}(t)\phi_{Jk}(x) = B\sum_{k=2-L}^{2^J-1} u_{J,k}(t)\frac{d^2}{dx^2}\phi_{Jk}(x) - C\sum_{k=2-L}^{2^J-1} u_{J,k}(t)\frac{d}{dx}\phi_{Jk}(x) + f(x,t). \quad (15)$$

To determine the coefficient $u_{J,k}$, we take the inner product of both sides of Equation (15) with $\phi_{Jl}$,

$$A\sum_{k=2-L}^{2^J-1} \dot{u}_{J,k}(t)\int_0^1 \phi_{J,k}(x)\phi_{Jl}(x)dx = B\sum_{k=2-L}^{2^J-1} u_{Jk}(t)\int_0^1 \phi''_{Jk}(x)\phi_{Jl}(x)dx - C\sum_{k=2-L}^{2^J-1} u_{Jk}(t)\int_0^1 \phi'_{Jk}(x)\phi_{Jl}(x)dx + \int_0^1 f(x,t)\phi_{Jl}(x)dx,$$
$$l = 2-L, 3-L, \ldots, 2^J-1, \quad (16)$$

We assume that $f(x, t) = h(t)z(x)$, where $z(x) = \sum_{i=0}^{m} a_i x^i$ , is a polynomial of degree $m$ in $x$, otherwise, we approximate $z$ by such a polynomial if necessary.

For simplicity, we define the following notations for integrals appearing in (16):

$$a_{kl}^J = \int_0^1 \phi_{Jk}(x)\phi_{Jl}(x)dx, \quad (17)$$

$$b_{kl}^J = \int_0^1 \phi'_{Jk}(x)\phi_{Jl}(x)dx, \quad (18)$$

$$c_{kl}^J = \int_0^1 \phi''_{Jk}(x)\phi_{Jl}(x)dx, \quad (19)$$

and

$$d_{ml}^J = \sum_{i=0}^{m} \int_0^1 a_i x^i\, \phi_{Jl}(x)dx. \quad (20)$$

The above integrals can be evaluated by the algorithms has been described in (Ming-quayer [17]). To see how they are related to the integrals defined in previous section, we substitute $\phi_{Jk}(x) = 2^{J/2}\phi(2^J x - k)$. Consequently, the integrals in (17)-(20) can be finally written as:

$$\begin{aligned} a_{kl}^J &= 2^J \int_0^1 \phi(2^J x - k)\phi(2^J x - l)dx \\ &= \int_{-l}^{2^J-l} \phi(y-(k-l))\phi(y)dy \\ &= \int_0^{2^J-l} \phi(y-(k-l))\phi(y)dy - \int_0^{-l} \phi(y-(k-l))\phi(y)dy \\ &= \Gamma_{k-l}^0(2^J-l) - \Gamma_{k-l}^0(-l), \end{aligned} \tag{21}$$

$$\begin{aligned} b_{kl}^J &= 2^{2J} \int_0^1 \phi'(2^J x - k)\phi(2^J x - l)dx \\ &= 2^J \int_{-l}^{2^J-l} \phi'(y-(k-l))\phi(y)dy \\ &= 2^J \left[\int_0^{2^J-l} \phi'(y-(k-l))\phi(y)dy - \int_0^{-l} \phi'(y-(k-l))\phi(y)dy\right] \\ &= 2^J \left[\Gamma_{k-l}^1(2^J-l) - \Gamma_{k-l}^1(-l)\right], \end{aligned} \tag{22}$$

$$\begin{aligned} c_{kl}^J &= 2^{3J} \int_0^1 \phi''(2^J x - k)\phi(2^J x - l)dx \\ &= 2^{2J} \int_{-l}^{2^J-l} \phi''(y-(k-l))\phi(y)dy \\ &= 2^{2J} \left[\int_0^{2^J-l} \phi''(y-(k-l))\phi(y)dy - \int_0^{-l} \phi''(y-(k-l))\phi(y)dy\right] \\ &= 2^{2J} \left[\Gamma_{k-l}^2(2^J-l) - \Gamma_{k-l}^2(-l)\right], \end{aligned} \tag{23}$$

and

$$\begin{aligned} d_{ml}^J &= \sum_{i=0}^{m} \int_0^1 a_i x^i \phi_{Jl}(x)dx \\ &= \sum_{i=0}^{m} \frac{a_i}{2^{(i+\frac{1}{2})J}} M_l^i\left(2^J\right). \end{aligned} \tag{24}$$

The algorithm for calculating $\Gamma_{k-l}^0, \Gamma_{k-l}^1, \Gamma_{k-l}^2$, and $M_l^m$ has been described (Ming-quayer [17]).

Using the notations defined in (17)–(20), we write the equation in (16) as:

$$A \sum_{k=2-L}^{2^J-1} a_{kl}^J \dot{u}_{J,k} = B \sum_{k=2-L}^{2^J-1} c_{kl}^J u_{J,k} - C \sum_{k=2-L}^{2^J-1} b_{kl}^J u_{J,k} + h(t) d_{ml}^J,$$
$$l = 2-L, 3-L, ..., 2^J - 1. \quad (25)$$

The above equations can be further put into the matrix-vector form:

$$A \Phi \dot{U} = B \Omega \mathbf{U} - C \Psi \mathbf{U} + h(t) \Upsilon, \quad (26)$$

where

$$\Phi = \left[a_{kl}^J\right]_{2-L \leq k, l \leq 2^J-1},$$
$$\Psi = \left[b_{kl}^J\right]_{2-L \leq k, l \leq 2^J-1},$$
$$\Omega = \left[c_{kl}^J\right]_{2-L \leq k, l \leq 2^J-1},$$
$$\Upsilon = [d_{ml}^J]_{2-L \leq l \leq 2^J-1},$$
$$\mathbf{U} = [u_{J,2-L}, u_{J,3-L}, \ldots, u_{J,2^J-1}]^t,$$

and

$$\dot{\mathbf{U}} = [\dot{u}_{J,2-L}, \dot{u}_{J,3-L}, \ldots, \dot{u}_{J,2^J-1}]^t,$$

where the exponent $t$ denotes the matrix transpose. The initial conditions for the differential equation (26) are derived from the initial conditions $u(x, 0)$ of the problem.

For the initial conditions $u(x, 0)$ given by equation (3), we consider the general case in which the initial condition is of the form $u(x, 0) = \eta(x)$, where as before $\eta(x)$ is assumed to be polynomial of degree $\nu$, otherwise we approximate it by such a polynomial. For this case the initial conditions $u_{J,k}(0)$ satisfy

$$u(x,0) = \sum_{k=2-L}^{2^J-1} u_{J,k}(0) \phi_{Jk}(x) = \eta(x). \quad (27)$$

We take the inner product of both sides of Equation (27) with $\phi_{Jl}$, $l \in Z$,

$$\sum_{k=2-L}^{2^J-1} u_{J,k}(0) \int_0^1 \phi_{J,k}(x) \phi_{J,l}(x) dx = \int_0^1 \eta(x) \phi_{Jl}(x) dx,$$
$$l = 2-L, 3-L, ..., 2^J - 1.$$

Hence, the initial condition $u_{J,k}(0)$ can be determined by solving the following linear system of algebraic equations:

$$\sum_{k=2-L}^{2^J-1} a_{kl}^J u_{J,k}(0) = d_{vl}^J, \tag{28}$$

where

$$d_{vl}^J = \int_0^1 \eta_1(x)\phi_{Jl}(x)dx, \quad l = 2-L, 3-L, \ldots, 2^J-1, \tag{29}$$

Having obtained the system of first order differential equations of (26) for $u_{J,k}$ with the initial conditions (28), we can utilize a numerical scheme to find the unknown coefficient vector **U**. We will solve the system by using the notation of the finite difference method $U_i = U(i\Delta t)$. Setting

$$\dot{\mathbf{U}}|_i = \frac{\mathbf{U}_{i+1} - \mathbf{U}_{i-1}}{\triangle t},$$

and the average value of **U** as

$$\mathbf{U}|_i = \frac{\mathbf{U}_{i+1} + \mathbf{U}_{i-1}}{2},$$

Equation (26) may be written in the form:

$$\mathbf{A}_1\mathbf{U}_{i+1} = \mathbf{A}_2\mathbf{U}_i + \mathbf{A}_3\,\Upsilon, \tag{30}$$

where

$$\mathbf{A}_1 = A\,\Phi - \frac{\triangle t}{2}(B\,\Omega - C\,\Psi),$$

$$\mathbf{A}_2 = A\,\Phi + \frac{\triangle t}{2}(B\,\Omega - C\,\Psi),$$

and

$$\mathbf{A}_3 = (\triangle t)\; h(t).$$

Equation (30) is a linear system of $(2^J+L-2)$ equations in $(2^J+L-2)$ unknown coefficients. This system may be easily solved by a variety of methods. In this paper we use *Q-R* method (Golub [11], Part-Enander [19], Shirvani [22]). By solving this system, we obtain an approximate solution at resolution level *J*. If we substitute $u_{J,k}(i\Delta t)$ in Equation (14), we can obtain an approximate solution to the problem (1)-(3) at any time point $i\Delta t$ .

## NUMERICAL EXAMPLES

For purposes of comparison, contrast and performance, examples with known solutions were chosen.

In the Wavelet-Galerkin solutions, Daubechies 6 wavelets are used because they give better results than those of lower degree wavelets and each example was run for a sequence of $J$ = 2, 3, 4, 5, 6, 7, 9. The non-homogeneous term has to be smooth, e.g., $f(x, t)$, has to be in some Sobolev space.

We use absolute error which is defined as:

$$\text{absolute error} = \left|u_{\text{exact solution}} - U_{\text{Wavelet-Galerkin}}\right|$$

Example 1. Consider the problem

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

If

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

subject to the boundary conditions

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

and the initial condition

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

then the exact solution is:

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

Table 1 shows the maximum absolute error at different time $t$ with $\Delta t = 0.001$ at different level $J$.

**Table 1. Maximum absolute error for example 1**

| | Level J=5 | Level J=7 | Level J=9 |
|---|---|---|---|
| **Time t =** 0.01 | 0.296E-06 | 0.294E-06 | 0.293E-06 |
| 0.1 | 0.275E-04 | 0.273E-05 | 0.271E-05 |
| 1.0 | 0.0014 | 0.314E-03 | 0.778E-04 |
| 1.5 | 0.0021 | 0.373E-03 | 0.107E-03 |

***Example*** 2. Consider the problem:

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

subject to the boundary conditions

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

and the initial condition

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

If

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

then the exact solution is

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

Table 2 shows the maximum absolute error at different time $t$ with $\Delta t = 0.001$ at different level J.

**Table 2. Maximum absolute error for example 2**

| | Level J=5 | Level J=7 | Level J=9 |
|---|---|---|---|
| **Time t =** 0.01 | 0.2475E-10 | 0.2475E-10 | 0.2475E-10 |
| 0.1 | 0.9178E-06 | 0.2328E-07 | 0.2328E-07 |
| 0.5 | 0.3107E-03 | 0.2638E-04 | 0.6038E-05 |
| 1.0 | 0.7547E-03 | 0.1584E-03 | 0.3672E-04 |

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

## CONCLUSION

As it has been shown in the paper, the proposed Wavelet-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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