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A new scheme for the solution of reaction diffusion and wave propagation problems

Ji Lin [a], Wen Chen [a,*], C.S. Chen [b]

[a] Center for Numerical Simulation Software in Engineering and Sciences, Department of Engineering Mechanics, Hohai University, No. 1 XiKang Road, Nanjing, Jiangsu 210098, China
[b] Department of Mathematics, University of Southern Mississippi, Hattiesburg, MS 39406, USA

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ABSTRACT

In this paper, a robust numerical scheme is presented for the reaction diffusion and wave propagation problems. The present method is rather simple and straightforward. The Houbolt method is applied so as to convert both types of partial differential equations into an equivalent system of modified Helmholtz equations. The method of fundamental solutions is then combined with the method of particular solution to solve these new systems of equations. Next, based on the exponential decay of the fundamental solution to the modified Helmholtz equation, the dense matrix is converted into an equivalent sparse matrix. Finally, verification studies on the sensitivity of the method's accuracy on the degree of sparseness and on the time step magnitude of the Houbolt method are carried out for four benchmark problems.

1. Introduction

Systems of reaction diffusion and wave propagation equations model a large number of physical phenomena in various scientific disciplines [1–6]. Analytical solutions to such problems are difficult or even impossible to construct whereby much information can be recovered from the use of numerical methods, as the finite elements method (FEM) [7,8], finite difference method (FDM)[9,10], boundary element method (BEM) [11,12], finite volume method (FVM) [13,14], spectral methods [15]. Although, these above-mentioned mesh-based numerical methods are dominated in engineering applications, some disadvantages also perplex the users such as the problems of mesh building, numerical quadrature and singular or hyper-singular integration. In recent decades, the co-called meshless or meshfree numerical schemes have been proposed to further circumvent these disadvantages [16–18].

The method of fundamental solution (MFS) [19–25] is one of the promising meshless numerical schemes which has rightfully received a great deal of attention by applied mathematicians and engineers in dealing with a variety of engineering problems. The basic concept of the MFS is to decompose the solutions of the given problems by the combination of the fundamental solutions of the governing equations with unknown proper intensities. The MFS was first proposed by Kupradze and Aleksidze [22] to approximate the solution of homogeneous elliptic-type partial differential equations. Furthermore, it was used for nonhomogeneous problems in combination with the method of particular solution (MPS) [26–28]. Prior to this study, it has been successfully applied to advection–diffusion equations, Burger's equations, advection equations and wave

* Corresponding author.
E-mail address: chenwen@hhu.edu.cn (W. Chen).

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equations. In this paper, we document the first attempt to apply the MFS for the solutions of reaction diffusion and wave propagation equations by employing the Houbolt finite difference scheme [29,30]. The Houbolt method is an implicit and unconditionally stable time-integration scheme [29]. The time-dependent loading of the system is discretized with the Houbolt method and corresponding set-up problem is solved by using the Euler scheme. Then the physical problem is converted into a nonhomogeneous modified Helmholtz equation at each time step, which is solved in this paper by using the coupled MFS-MPS method. The MPS and MFS satisfy the nonhomogeneous equation and the corresponding homogeneous equation, respectively. With the combination of the MFS and MPS, a truly meshless numerical scheme has been achieved. In the MFS–MPS, we need to solve two densely populated matrices, one is for the particular solution by the MPS, and the other is for homogeneous solution by the MFS. The development of the compactly supported radial basis function has made it possible for the resulted MPS matrix to be sparse.

It is known that the coefficient matrix resulted from the MFS discretization is densely populated and that the condition number is high [19,31]. Furthermore, for a large number of collocation points, it is expensive to solve. Direct solver for these types of matrices require $O(N^3)$ operations and $O(N^2)$ storage entries. Also, it is possible that an ill-conditioned system will result, whose solution will be either inaccurate or divergent, rendering the numerical simulation worthless [32]. It is also well-known that, the feature of the MFS matrix is in generally largely depended on the prescribed boundary conditions, the choice of the fictitious boundary and the wave-number. Based on the nature exponential decay of the fundamental solutions [33] of the modified Helmholtz operator, the elements of the MFS matrix would be very small. The discrepancy between the maximum and minimum values in the MFS matrix becomes wide apart. For large wave-number, most of the MFS matrix elements have small values, which can be neglected in the computing process. As a result, the original densely populated matrix becomes a sparse system in order to reduce the computational cost and circumvent the ill-conditioned feature. The purpose of this paper is to illustrate the sensitivity of the method's accuracy on the degree of sparseness and on the time step magnitude of the Houbolt method for reaction diffusion and wave propagation problems.

The rest of the paper is organized as follows. In Section 2, governing equations and the Houbolt method are introduced. The method of fundamental solution combined with the matrix sparseness technique and the method of particular solution are presented in Section 3 and Section 4 respectively. Four numerical examples are employed to verify the accuracy and efficiency compared with the analytical solutions or solutions obtained by the FEM. Section 5 concludes this study with some remarks.

2. Governing equations and the Houbolt method

The governing equations of time-dependent reaction diffusion and wave propagation problems can be written as

$$\Delta u - cu = \frac{\partial u}{\partial t} + f, \quad t > 0, \tag{1}$$

$$\Delta u - cu = \frac{\partial^2 u}{\partial t^2} + f, \quad t > 0, \tag{2}$$

where Δ is the Laplace operator, $u = u(x,t)$ is a state variable at position x, time t, $x = [\mathrm{x}_1 \quad \mathrm{x}_2]$ for two-dimensional problem, $x = [\mathrm{x}_1 \quad \mathrm{x}_2 \quad \mathrm{x}_3]$ for three-dimensional problem, and c is a constant.

In order to deal with the time-dependent terms of Eqs. (1) and (2), the Houbolt method is selected to discretize the time domain. The Houbolt method is a three-steps implicit and unconditionally stable time-integration scheme based on the third-order interpolation. The difference formulae with respect to time t in the Houbolt method can be approximated as follows:

$$\left\{\frac{\partial u}{\partial t}\right\}^{n+1} \approx \frac{1}{6\delta t}(11u^{n+1} - 18u^n + 9u^{n-1} - 2u^{n-2}), \tag{3}$$

$$\left\{\frac{\partial^2 u}{\partial t^2}\right\}^{n+1} \approx \frac{1}{\delta t^2}(2u^{n+1} - 5u^n + 4u^{n-1} - u^{n-2}), \tag{4}$$

here δt is the time interval with time meshing $t_n = n \times \delta t$ (δt is the time step size) and $u^n = u(*, t_n)$, the superscripts of u represent the time level. By substituting $\partial u/\partial t$ and $\partial^2 u/\partial t^2$ from Eqs. (3) and (4), respectively, into Eqs. (1) and (2), we obtain the following equations:

$$\Delta u^{n+1} - cu^{n+1} - \frac{11}{6\delta t}u^{n+1} = \frac{1}{6\delta t}(-18u^n + 9u^{n-1} - 2u^{n-2}) + f^{n+1}, \tag{5}$$

$$\Delta u^{n+1} - cu^{n+1} - \frac{2}{\delta t^2}u^{n+1} = \frac{1}{\delta t^2}(-5u^n + 4u^{n-1} - u^{n-2}) + f^{n+1}, \tag{6}$$

To deal with the setup problem of time stepping, the first order Euler scheme is used to obtain u^{n-1} and u^{n-2} as follows:

$$u^{n-1} = u(x,t)|_{t=0} - \delta t \left.\frac{\partial u(x,t)}{\partial t}\right|_{t=0}, \quad n \le 2, \tag{7}$$

$$u^{n-2} = u(x,t)|_{t=0} - 2\delta t \left.\frac{\partial u(x,t)}{\partial t}\right|_{t=0}, \quad n \le 2. \tag{8}$$