ISSN 1746-7659, England, UK
Journal of Information and Computing Science
Vol. 2, No. 4, 2007, *pp*. 243-251

High-order Difference Methods for Multi-scale Ground Water Flow *

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(*Received January 17 2007, accepted April 22 2007*)

Abstract. In this paper, we develop several high-order finite difference schemes to simulate ground water flow in heterogeneous porous media. Our main purpose is to demonstrate that the high-order method can be used to resolve the fine scales efficiently for flow in heterogeneous porous media. The effectiveness of this approach is illustrated by two examples and detailed comparison with the classic second-order method and homogenization technique.

Keywords: Ground water, high-order scheme, heterogeneous media.

1. Introduction

One major difficult in analyzing ground water flow and solute transport is mainly caused by the heterogenity of subsurface formations spanning many scales. Though many progress have been made in the past three decades in ground water simulation in highly heterogeneous media (Dagan, 1989; Zhang, 2002), our ability remains limited even with modern super-computers.

Many multiscale methods have been introduced in recent years, such as the multiscale finite element method (Hou et a), 1997; Hughes et al, 1998), methods based on the homogenization theory (Dylcaar et al, 1992), upscaling methods (Arbogast, 2003), and the heterogeneous niultiscale methods (E et al, 2003). The central goal of these methods is to efficiently capture the large scale behavior of the solution without resolving the small scale features. However, in some cases we have to obtain very accurately the small scale effect on the large scale applications, then we have to resolve all the fine scales as accurate as possible. Some recent direct simulations of flow and transport in heterogeneous porous media are reported (Ababou et al, 1989; Burr et al, 1994; Tompson, 1993). But they are all based on low-order schemes. Considering the success of high-order methods for direct simulation of turbulent flows and wave propogation problems with a range of spatial scales (Lele, 1992; Gaitonde et al, 1998; Li, 2005; Li et al, 2006), our goal in this paper is to develop high-order difference schemes for directly simulating groundwater flow problems in heterogeneous media. One major advantage of high-order methods is that much fewer mesh points are needed in order to achieve the same accuracy compared to widely adopted low-order methods in ground water modeling (Wang et al 1982; Zheng et al, 2002), which fact makes directly solving multiscale problems possible by using high-order methods. For simplicity, in this paper we only focus on the ground water flow problem

$$S_s \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(K_x \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(K_y \frac{\partial u}{\partial y}) + R$$

where u is the hydraulic head, K_x and K_y are the hydraulic condurtivitv in x and y direction, respectively, S is the specific storage, and R is the fluid sink/source term. More complicated problems will he investigated in our future work.

The remainder of this paper is organized as follows. In Section 2, we focus on the development of some high-order difference schemes. Then we test our high-order schemes for ground water flow problems

* This work was partially supported by the National Science Foundation under grant INT-0328186 and Grant No. 0447416 (Nevada NSF EPSCoR Ring True Program III).

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with highly oscillatory hydraulic conductivity. Section 4 is reserved for some conclusions.

2. The algorithms

For simplicity, we focus on the one-dimensional case

$$\frac{\partial}{\partial x}(K\frac{\partial u}{\partial x}) = R \quad 0 < x < 1 \tag{1}$$

$$u|_{x=0} = u_l, \quad u|_{x=1} = u_r \tag{2}$$

considering that analytical solutions in higher dimensions are difficult to obtain for accuracy comparison. We assume a uniform mesh, consisting of N points, i.e., $x_i = (i-1)\Delta x$, $i = 1, 2, \cdots N$, where the mesh size $\Delta x = 1/(N-1)$, and $x_{i+1/2}$ denote the mid-points. We can solve (1)-(2) by a classic second-order difference scheme

$$K_{i+1/2}\frac{u_{i+1}-u_i}{\Delta x} - K_{i-1/2}\frac{u_i - u_{i-1}}{\Delta x} = \Delta x R_i \quad 2 \le i \le N-1,$$

where we denote u_i the approximate solution of u at point x_i , $K_{i+1/2} = K(x_{i+1/2})$, $R_i = R(x_i)$. To construct a high-order difference scheme, we integrate (1) in x over the interval $[x_{i-1/2}, x_{i+1/2}], \quad i = 2, 3, \cdots N-1$, we obtain

$$K_{i+1/2}\frac{\partial u}{\partial x}\Big|_{i+1/2} - K_{i-1/2}\frac{\partial u}{\partial x}\Big|_{i-1/2} = \int_{x_i-1/2}^{x_i+1/2} R(x)dx \tag{3}$$

where the derivatives $\partial u/\partial x$ at the mid-points will be approximated by high-order difference formulas given below. The integral is approximated by the four-point Gaussian quadrature, hence the global accuracy is dominated by the derivative errors.

2.1. The fourth-order scheme

For: $i = 2, 3, \cdots N-1$, we have (Lele, 1992, equation (B.1.3))

$$\frac{\partial u}{\partial x}\Big|_{i+1/2} = b\frac{u_{i+2}-u_{i-1}}{3\Delta x} + a\frac{u_{i+1}-u_i}{\Delta x} \tag{4}$$

where a=9/8, b= -1/8. This formula has a truncation error $\frac{9}{1920}(\Delta x)^4 u^{(5)}$.

For the near boundary points $x_{3/2}, x_{N-1/2}$, special formulas are needed. For fourth-order accuracy, we have (Gaitonde et al, 1998, Table 2.11)

$$\frac{\partial u}{\partial x}\Big|_{3/2} = [a_1u_1 + a_2u_2 + a_3u_3 + a_4u_4 + a_5u_5]/(\Delta x)$$

$$\frac{\partial u}{\partial x}\Big|_{N-1/2} = -[a_1u_N + a_2u_{N-1} + a_3u_{N-2} + a_4u_{N-3} + a_5u_{N-4}]/(\Delta x)$$

where

$$a_1 = -\frac{22}{24}, a_2 = \frac{17}{24}, a_3 = \frac{3}{8}, a_4 = -\frac{5}{24}, a_5 = \frac{1}{24}$$

For third-order accracy, we have (Gaitonde et al, 1998, Table 2.11)

$$\frac{\partial u}{\partial x}\Big|_{3/2} = [b_1u_1 + b_2u_2 + b_3u_3 + b_4u_4]/(\Delta x)$$

$$\frac{\partial u}{\partial x}\Big|_{N-1/2} = -[b_1u_N + b_2u_{N-1} + b_3u_{N-2} + b_4u_{N-3}]/(\Delta x)$$

where

$$b_1 = -\frac{23}{24}, b_2 = \frac{7}{8}, b_3 = \frac{1}{8}, b_4 = -\frac{1}{24}.$$

To distinguish different order schemes, we use the simple notation b-i-b for a scheme with *i*th-order for interior points, and *b*th-order for near boundary points. For example, 4-4-4 denotes a scheme with fourth-ordar for both interior and near boundary points.

2.2. The sixth-order schcme

For $i = 4, 5, \cdots, N-3$, we have (Lele, 1992, equation (B.1.4))

$$\left.\frac{\partial u}{\partial x}\right|_{i+1/2} = \tilde{c}\frac{u_{i+3} - u_{i-2}}{5\Delta x} + \tilde{b}\frac{u_{i+2} - u_{i-1}}{3\Delta x} + \tilde{a}\frac{u_{i+1} - u_i}{\Delta x} \quad (5)$$

Where $\tilde{a} = 150/128, \tilde{b} = -25/128, \tilde{c} = 3/128$. This formula has a truncation error $\frac{75}{107520}(\Delta x)^6 u^{(7)}$

Due to wider stencils, special fommla are needed for the near boundary points $x_{i+1/2}, \quad i = 2, 3, \cdots, N-1$. For fifth-order accuracy, we have (Gaitonde et al, 1998, Table 2.11)

$$\left.\frac{\partial u}{\partial x}\right|_{3/2} = [\tilde{a}_1 u_1 + \tilde{a}_2 u_2 + \tilde{a}_3 u_3 + \tilde{a}_4 u_4 + \tilde{a}_5 u_5 + \tilde{a}_6 u_6]/(\Delta x)$$

$$\left.\frac{\partial u}{\partial x}\right|_{N-1/2} = -[\tilde{a}_1 u_N + \tilde{a}_2 u_{N-1} + \tilde{a}_3 u_{N-2} + \tilde{a}_4 u_{N-3} + \tilde{a}_5 u_{N-4} + \tilde{a}_6 u_{N-5}]/(\Delta x)$$

where

$$\tilde{a}_1 = -\frac{563}{640}, \tilde{a}_2 = \frac{67}{128}, \tilde{a}_3 = \frac{143}{192}, \tilde{a}_4 = -\frac{37}{64}, \tilde{a}_5 = \frac{29}{128}, \tilde{a}_6 = \frac{71}{1920}$$

Now we shall derive the fifth-order sheme for nodes $x_{i+1/2}, \quad i = 3, \cdots, N-2$. We assume

$$\left.\frac{\partial u}{\partial x}\right|_{5/2} = [\tilde{b}_1 u_1 + \tilde{b}_2 u_2 + \tilde{b}_3 u_3 + \tilde{b}_4 u_4 + \tilde{b}_5 u_5 + \tilde{b}_6 u_6]/(\Delta x)$$

where the coefficients $\tilde{b}_i, i = 1, 2, \cdots, 6$, can be determined by Taylor expansion to the order of $O(\Delta x)^5$:

$$\tilde{b}_1 + \tilde{b}_2 + \tilde{b}_3 + \tilde{b}_4 + \tilde{b}_5 + \tilde{b}_6 = 0$$

$$(-\frac{3}{2})^1\tilde{b}_1 + (-\frac{1}{2})^1\tilde{b}_2 + (\frac{1}{2})^1\tilde{b}_3 + (\frac{3}{2})^1\tilde{b}_4 + (\frac{5}{2})^1\tilde{b}_5 + (\frac{7}{2})^1\tilde{b}_6 = 1$$

$$(-\frac{3}{2})^2\tilde{b}_1 + (-\frac{1}{2})^2\tilde{b}_2 + (\frac{1}{2})^2\tilde{b}_3 + (\frac{3}{2})^2\tilde{b}_4 + (\frac{5}{2})^2\tilde{b}_5 + (\frac{7}{2})^2\tilde{b}_6 = 0$$

$$(-\frac{3}{2})^3\tilde{b}_1 + (-\frac{1}{2})^3\tilde{b}_2 + (\frac{1}{2})^3\tilde{b}_3 + (\frac{3}{2})^3\tilde{b}_4 + (\frac{5}{2})^3\tilde{b}_5 + (\frac{7}{2})^3\tilde{b}_6 = 0$$

$$(-\frac{3}{2})^4\tilde{b}_1 + (-\frac{1}{2})^4\tilde{b}_2 + (\frac{1}{2})^4\tilde{b}_3 + (\frac{3}{2})^4\tilde{b}_4 + (\frac{5}{2})^4\tilde{b}_5 + (\frac{7}{2})^4\tilde{b}_6 = 0$$

$$(-\frac{3}{2})^5\tilde{b}_1 + (-\frac{1}{2})^5\tilde{b}_2 + (\frac{1}{2})^5\tilde{b}_3 + (\frac{3}{2})^5\tilde{b}_4 + (\frac{5}{2})^5\tilde{b}_5 + (\frac{7}{2})^5\tilde{b}_6 = 0$$

which gives the solution

$$\tilde{b}_1 = \frac{71}{1920}, \tilde{b}_2 = -\frac{141}{128}, \tilde{b}_3 = \frac{69}{64}, \tilde{b}_4 = \frac{1}{192}, \tilde{b}_5 = -\frac{3}{128}, \tilde{b}_6 = \frac{3}{640}.$$

Similarly, it is easy to prove the following fifth-order scheme

$$\left.\frac{\partial u}{\partial x}\right|_{N-3/2} = -[\tilde{b}_1 u_N + \tilde{b}_2 u_{N-1} + \tilde{b}_3 u_{N-2} + \tilde{b}_4 u_{N-3} + \tilde{b}_5 u_{N-4} + \tilde{b}_6 u_{N-5}]/(\Delta x)$$

To distinguish different order schemes, we use simple notation b-b-i-b-b for a scheme with *i*th-order for interior points, and *b*th-order for near boundary points, For example, 5-5-6-5-5 denotes a scheme with sixth-order for interior points, and fifth-order for near boundary points.

3. Numerical examples

Example 1. Here we solve the problem (1)-(2) with

$$K(x, x/\varepsilon) = 1/(2 + A\sin\frac{2\pi x}{\varepsilon}), u_i = 2, u_r = 1, R = 1.$$

Using integration by parts, we can easily obtain the exact solution of (1)-(2)

$$u_{ex}(x) = x^2 + 2Cx - A\frac{\varepsilon}{2\pi}x\cos(\frac{2\pi x}{\varepsilon}) + A(\frac{\varepsilon}{2\pi})^2\sin(\frac{2\pi x}{\varepsilon}) - AC\frac{\varepsilon}{2\pi}\cos(\frac{2\pi x}{\varepsilon}) + D$$

where $C = A\varepsilon/4\pi - 1, D = 2 + AC\varepsilon/2\pi$, the coefficient K is highly oscillatory, an example is shown in Fig.1 for the case of A = 1.9, $\varepsilon = 0.1$.

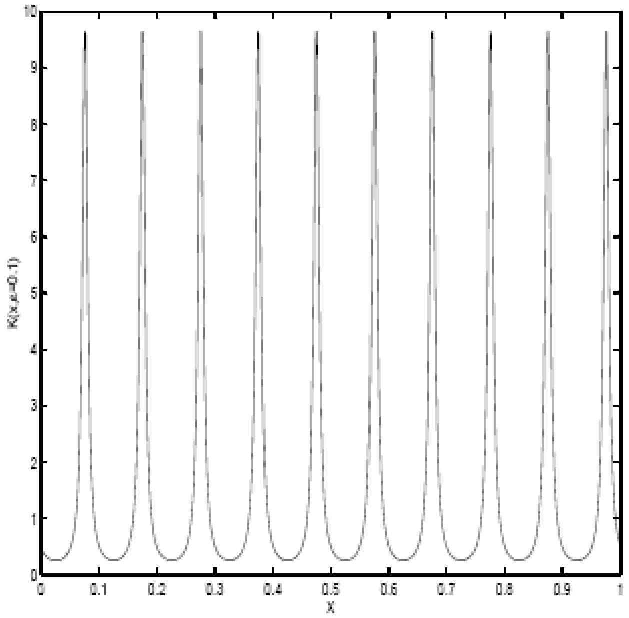

Fig. 1 The plot for the coefficient K of Example 1 with A = 1.9, $\varepsilon = 0.1$

We solved the problem with A = 1.9, $\varepsilon = 0.1, 0.01$, by schemes of different orders. The convergence rate is estimated by $r = \log(e_N / e_{2N})/\log(2)$, where e_N, e_{2N} denote the maximum errors achieved with N and $2N$ uniform subintervals. Detailed convergence rates and CPU time used for different. schemes are presented in Tables 1 and 2 for $\varepsilon = 0.1, 0.01$, respectively.

Our numerical results show clearly that the high-order schemes can achieve several order magnitude better than the classic second-order scheme with the same number of mesh points (see Fig.2). To achieve a fixed accuracy, the high-order schemes need much less mesh points than the second-order scheme (see Fig.3). For example, with $\varepsilon = 0.1$, the second-order scheme's maximum error is 5.7227e-7 using N = 4001 points, while both 4-4-6-4-4 and 5-5-6-5-5 schemes has the maximum error 2.2700e-7 with only N = 251 points, This fact shows that the high-order schemes is very efficient and accurate for solving ground water flow problems in heterogeneous media directly.

Table 1. Maximum errors for Example 1 with $\varepsilon = 0.1$

Numbeer of points	Maximum error	Convergence rate	CPU time(in seconds)
2^{nd}-order scheme			
N=251	1.4656e-4	*	0.50
N=501	3.6617e-5	2.0009	0.60
N=1001	9.1570e-6	1.9996	0.88
N=2001	2.2891e-6	2.0001	1.76
N=4001	5.7227e-7	2.000	4.17
3-4-3 scheme			
N=251	4.9118e-6	*	0.77
N=501	3.2507e-7	3.9174	0.99
N=1001	2.0676e-8	3.9747	1.71
N=2001	1.3007e-9	3.9906	3.41
N=4001	1.1199e-10	3.5378	8.57
4-4-4 scheme			
N=251	5.3859e-7	*	0.77
N=501	5.5224e-8	3.2858	1.10
N=1001	3.8712e-9	3.8344	1.92
N=2001	2.4978e-10	3.9541	3.96
N=4001	1.2129e-10	*	11.32
4-4-6-4-4 scheme			
N=251	2.3379e-7	*	0.77
N=501	4.2398e-9	5.7851	1.15
N=1001	6.8838e-11	5.9446	2.08
N=2001	4.4063e-11	*	4.56
N=4001	5.3873e-11	*	12.74
5-5-6-5-5 scheme			
N=251	2.2700e-7	*	0.72
N=501	4.1447e-9	5.7753	1.37
N=1001	6.7752e-11	5.9349	2.47
N=2001	4.4182e-11	*	5.38
N=4001	5.3873e-11	*	14.28

Table 2. Maximum errors for Example 1 with $\varepsilon = 0.01$

Numbeer of points	Maximum error	Convergence rate	CPU time(in seconds)
2^{nd}-order scheme			
N=251	0.0017	*	0.49
N=501	3.7476e-4	2.1815	0.61
N=1001	9.9831e-5	1.9084	0.99
N=2001	2.4742e-5	2.0125	1.70
N=4001	6.1723e-6	2.0031	4.18
3-4-3 scheme			
N=251	0.0024	*	0.60
N=501	7.9233e-5	4.9208	0.94
N=1001	1.5846e-5	2.3220	1.65
N=2001	1.2253e-6	3.6929	3.35
N=4001	8.0814e-8	3.9244	8.57
4-4-4 scheme			
N=251	0.0031	*	0.72
N=501	3.0104e-4	3.3642	1.10
N=1001	1.0259e-5	4.8750	2.70
N=2001	1.9291e-7	5.7328	3.96
N=4001	1.3900e-8	3.7948	11.54
4-4-6-4-4 scheme			
N=251	0.0032	*	0.71
N=501	2.8470e-4	3.4906	1.09
N=1001	1.6937e-6	7.3931	2.09
N=2001	8.6371e-8	4.2935	4.56
N=4001	1.6422e-9	5.7168	13.79
5-5-6-5-5 scheme			
N=251	0.0032	*	0.77
N=501	2.8564e-4	3.4858	1.48
N=1001	1.5199e-6	7.5541	2.47
N=2001	8.3970e-8	4.1780	5.28
N=4001	1.6073e-9	5.7072	14.39

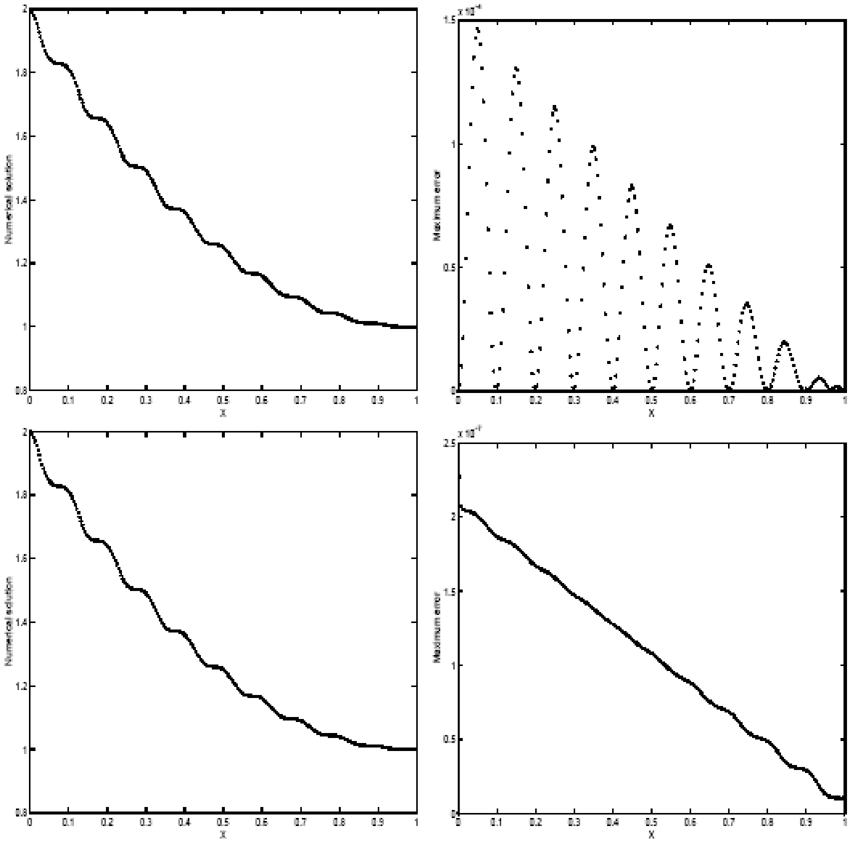

Fig. 2. Example 1 with $\varepsilon = 0.01$. Top row shows the numerical solution (Left) and piontwise maximum error (Right) obtained with the 2nd-order scheme with N=251 points. Bottom row shows the numerical solution (Left) and pointwise maximun error (Right) obtained with the 5-5-6-5-5 scheme with N=251 points.

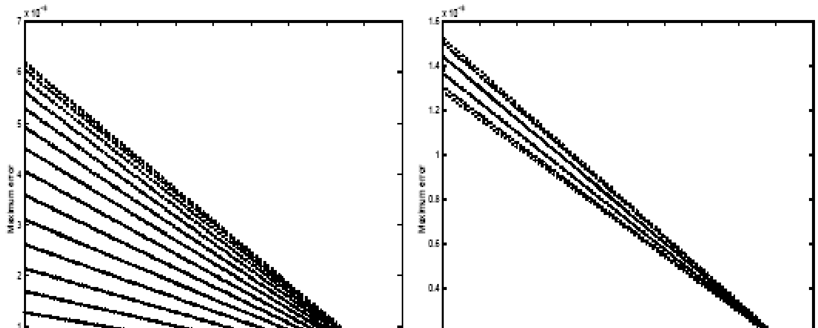

Fig. 3. Example 1 with $\varepsilon = 0.01$. Pointwise maximum errors obtained by the 2nd-scheme with N=4001 points (left) and by the 5-5-6-5-5 scheme with N=1001 points (Right).

Finally, we want to mention that the homogenized problem (Avellaneda et al, 1991, p.695) of (1)-(2) is:

$$\frac{\partial}{\partial x}\left(\overline{K}\frac{\partial \overline{u}}{\partial x}\right) = R \quad 0 < x < 1 \tag{6}$$

$$\overline{u}\Big|_{x=0} = u_l, \quad \overline{u}\Big|_{x=1} = u_r \tag{7}$$

Where $\overline{K} = [\int_0^1 \frac{1}{K(x,y)} dy]^{-1}$. Hence for our example, we can easily check that

$$\overline{K} = \left(\int_0^1 (2 + A\sin 2\pi y) dy\right)^{-1} = 1/2$$

and the homogenized solution

$$\bar{u}(x) = x^2 - 2x + 2$$

And the Darcy velocity $\bar{q} = -\bar{K}\,\partial\bar{u}/\partial x = -(x+C)$, which shows that the maximum errors between the homogenized and exact solution (or Darcy velocity) will be

$$\sup_{0\le x\le 1}\left|u_{ex}(x) - \bar{u}(x)\right| \le C\varepsilon, \quad \sup_{0\le x\le 1}\left|q_{ex}(x) - \bar{q}(x)\right| \le C\varepsilon .$$

This means that the homogenized problem is not a very accurate approximation to the original multiscale problem. We demonstrate this by solving the homogenized problem with $\varepsilon = 0.1$ using 5-5-6-5-5 scheme with 251 points, the homogenized solution and the maximum errors between the homogenized and exact solution are presented in Fig.4.

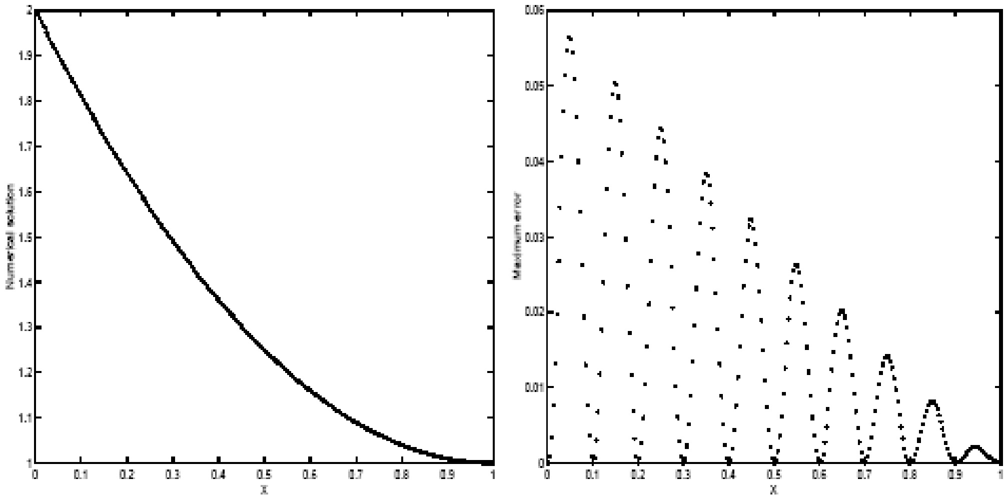

Fig. 4. The homogenized solution (Left) and maximum errors (Right) between the homogenized and exact solution obtained with the 5-5-6-5-5 scheme with N=251 points and $\varepsilon = 0.1$.

Example 2. In this example, we consider a case with multi-scale hydraulic conductivity, i.e., we solve the problem (1)-(2) with u_l=2, u_r=1, R=1, and

$$K(x,\varepsilon) = 1/(5 + A_1\sin(2\pi f_1 x) + A_2\sin(2\pi f_2 x) + A_3\sin(2\pi f_3 x))$$

Using integration by parts, we can easily obtain the exact solution of (1)-(2)

$$\begin{aligned} u_{ex}(x) &= \frac{5}{2}x^2 + 5Cx + D \\ &+ A_1[-\frac{1}{2\pi f_1}x\cos(2\pi f_1 x) + (\frac{1}{2\pi f_1})^2\sin(2\pi f_1 x) - \frac{C}{2\pi f_1}\cos(2\pi f_1 x)] \\ &+ A_2[-\frac{1}{2\pi f_2}x\cos(2\pi f_2 x) + (\frac{1}{2\pi f_2})^2\sin(2\pi f_2 x) - \frac{C}{2\pi f_2}\cos(2\pi f_2 x)] \\ &+ A_3[-\frac{1}{2\pi f_3}x\cos(2\pi f_3 x) + (\frac{1}{2\pi f_3})^2\sin(2\pi f_3 x) - \frac{C}{2\pi f_3}\cos(2\pi f_3 x)] \end{aligned}$$

where

$$C = \frac{1}{5}(\frac{A_1}{2\pi f_1} + \frac{A_2}{2\pi f_2} + \frac{A_3}{2\pi f_3} - \frac{7}{2}), \quad D = 2 + C(\frac{A_1}{2\pi f_1} + \frac{A_2}{2\pi f_2} + \frac{A_3}{2\pi f_3}).$$

An example of coefficient K is shown in Fig.5 for the case of $A_1 = A_3 = 1$, $A_2 = 2$, $f_1 = 2$, $f_2 = 8$, $f_3 = 32$.

We performed many experiments with different order schemes and number of mesh points. Our results show once more that the high-order schemes can achieve several order magnitude hotter than the classic second-order scheme with the same number of mesh points. Some representative results are provided in Table 3 and Fig. 6.

4. Conclusions

In summary, we have developed both fourth- and sixth-order difference methods for solving heterogeneous ground water flow problems. The high-order methods can achieve the same accuracy with less nodal points compared to the classical low-order methods, which fact makes high-order methods very attractive for problem with multiscales. Two one-dimensional examples containing multiple scales are presented and the results demonstrate the efficiency of the high-order methods through detailed comparisons with the second-order methods and the homogenized solution. The high-order methods can be extended to both higher dimension problems and time-dependent problems, see (Gaitonde et al. 1998; Li , 2005: Li et al, 2006) and references therein. More complex ground water flows in heterogeneous media will be investigated and reported in our future work.

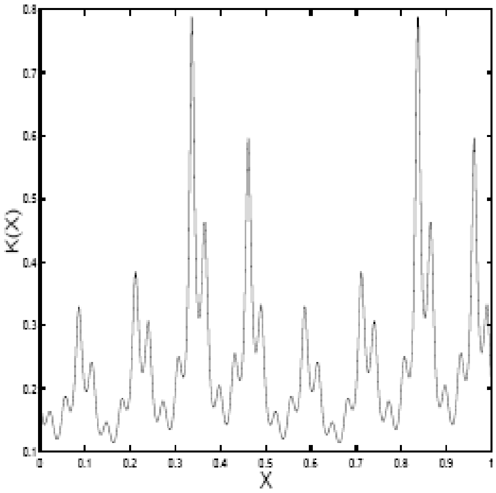

Fig. 5. The plot for the coefficient *K* of example 2 with $A_1 = A_3 = 1$, $A_2 = 2$, $f_1 = 2$, $f_2 = 8$, $f_3 = 32$.

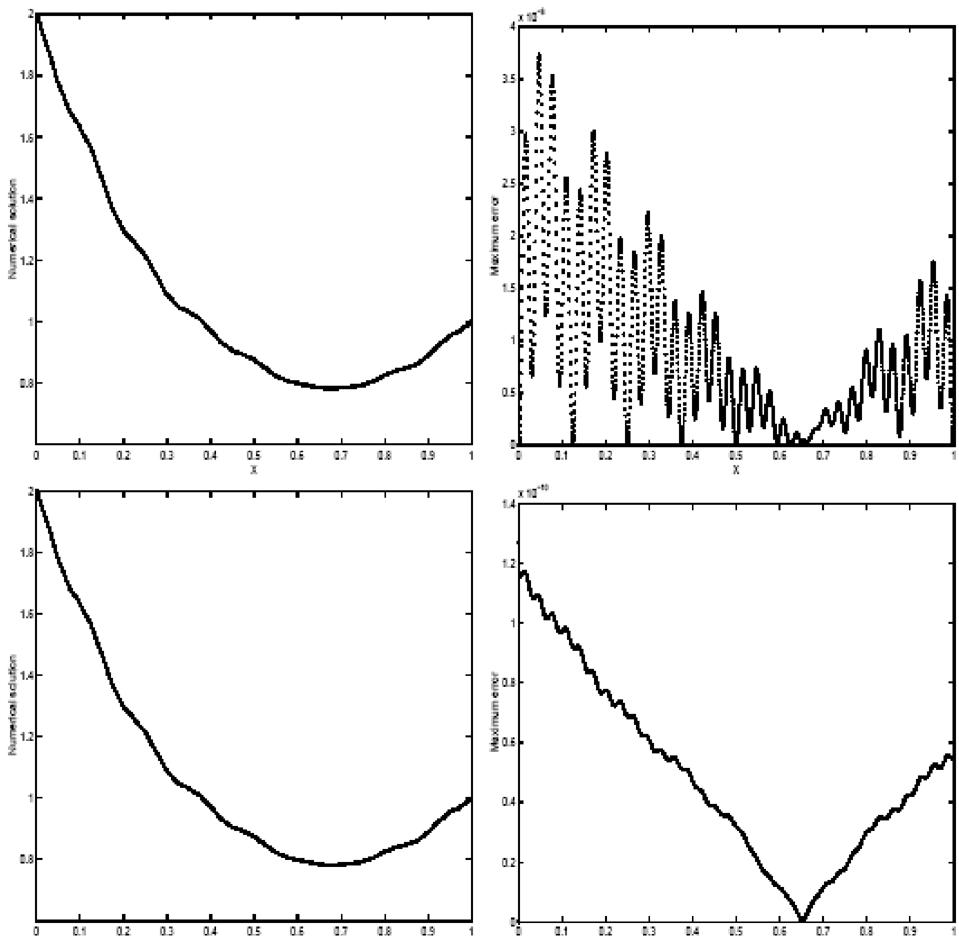

Fig. 6. Example 2. Top row shows the numerical solution (Left) andpointwise maximum error (Right) obtained with the 2nd-order scheme with *N*=2001 points. Bottom row shows the numerical solution (Left) and pointwise maxiumum error (Right) obtained with the 5-5-6-5-5 scheme with *N*=2001 points.

Table 3. Maximum errors for Example 2

Number of points	Maximum error	Convergence rate	CPU time(in seconds)
2^{nd}-order scheme			
N=251	2.4070e-4	*	0.50
N=501	5.9572e-5	2.0145	0.66
N=1001	1.4935e-5	1.9959	0.99
N=2001	3.7315e-6	2.0009	1.81
N=4001	9.3275e-7	2.0002	4.28
5-5-6-5-5 scheme			
N=251	4.7953e-6	*	0.71
N=501	3.2590e-7	3.8791	1.15
N=1001	7.4322e-9	5.4545	2.25
N=2001	1.2681e-10	5.8730	4.78
N=4001	1.2062e-11	3.3941	12.80

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