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# Solving the Sod Shock Tube Problem Using Localized Differential Quadrature (LDQ) Method

**Zhi Zong[1,2], Zhangrui Li[1*] and Jing Dong[1]**

*1. Department of Naval Architecture and Ocean Engineering, Dalian University of Technology, Dalian 116023, China*
*2. State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology, Dalian 116023, China*

**Abstract:** The localized differential quadrature (LDQ) method is a numerical technique with high accuracy for solving most kinds of nonlinear problems in engineering and can overcome the difficulties of other methods (such as difference method) to numerically evaluate the derivatives of the functions. Its high efficiency and accuracy attract many engineers to apply the method to solve most of the numerical problems in engineering. However, difficulties can still be found in some particular problems. In the following study, the LDQ was applied to solve the Sod shock tube problem. This problem is a very particular kind of problem, which challenges many common numerical methods. Three different examples were given for testing the robustness and accuracy of the LDQ. In the first example, in which common initial conditions and solving methods were given, the numerical oscillations could be found dramatically; in the second example, the initial conditions were adjusted appropriately and the numerical oscillations were less dramatic than that in the first example; in the third example, the momentum equation of the Sod shock tube problem was corrected by adding artificial viscosity, causing the numerical oscillations to nearly disappear in the process of calculation. The numerical results presented demonstrate the detailed difficulties encountered in the calculations, which need to be improved in future work. However, in summary, the localized differential quadrature is shown to be a trustworthy method for solving most of the nonlinear problems in engineering.
**Keywords:** localized differential quadrature; Sod shock tube; numerical oscillations; artificial viscosity
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## 1 Introduction

Differential quadrature (DQ) is a simple and advanced numerical method for evaluating derivatives of a sufficiently smooth function, proposed by Bellman *et al*. (1972). Its core idea is to approximate the derivatives at a point using a weighted sum of function values at a set of selected grid points. As shown by Shu (2000), DQ is a global method, equivalent to higher-order finite difference scheme. However, realized from the very beginning that DQ is not efficient when the number of grid points is large (Civian and Sliepcevich, 1984), it is sensitive to grid distribution and requires that the number of grid points cannot be too large. To improve this situation, localized differential quadrature to a small neighbourhood was introduced by Zong and Lam (2002), it succeeded in solving the 2-D wave equation and the wave propagation in one and two dimensional poroelastic media (Lam *et al*., 2004).

DQ is a high accuracy numerical method for solving nonlinear problems. Its applicability to solving equations of shock behavior is, however, yet to be examined. In this paper we apply localized differential quadrature (LDQ) to Sod shock tube problem as an instance to assess the capability of DQ method for solving shock propagations.

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***Corresponding author Email:** lizhangruix@yahoo.com.cn


The Sod shock tube problem, which is a simple one dimensional model of gas dynamics, was first introduced by Sod (1978). It is a peculiar case of a wider class of problems called Riemann problem. For a detailed discussion on the shock-tube problem the reader is referred to the book by Courant and Friedrichs (1985) and by Toro (1999). Even though this is such a simple problem with a simple solution, it is very difficult to simulate numerically. The reason for this is that the derivative is infinite at the discontinuity: mathematically it is a delta function. The solution of the Sod shock tube problem has been challenging the numerical methods for many years. This problem can be solved, approximately, by some kinds of difference methods proposed by Godunov, Lax-Wendroff, MacCormack, Rusanov, to say a few, or the Upwind Scheme (Sod, 1978). But typically these schemes produce oscillations behind a shock. All the finite difference schemes have numerical diffusion, dispersion, or both due to the truncation error. Busegnies *et al*. (2007) adopted smoothed particle hydrodynamics (SPH) to solve the shock tube problem, in which they introduced the artificial viscosity in the process of calculation.

The exact solution of the Sod shock tube problem is an invaluable reference solution that is useful in accessing the performance of numerical methods and to check the correctness of program in early stages of development. In this paper the exact solution is obtained by the exact Riemann solver for the Euler equation. For more details, please refer to Toro (1999).

The equations of fluid dynamics are mathematical statements of three fundamental physical principles:

- Mass is conserved.
- $F = ma$, i.e., Newton's second law.
- Energy is conserved.

The one-dimensional equations for the fluid dynamics of a gas can be written in conservation form as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \tag{1}$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial x}(\rho u^2 + p) = 0 \tag{2}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}(u(E+p)) = 0 \tag{3}$$

where $\rho$ is the density of the fluid, kg/m$^3$; $u$ the fluid velocity, m/s; $E$ the energy per unit volume (length), J/kg; $p$ the fluid pressure, Pa; $t$ the time, s; and $x$ the distance, m.

We need one more equation to close the system. This is the equation of state:

$$p = (\gamma - 1)(E - \frac{1}{2}\rho u^2) \tag{4}$$

# 2 Finding derivation using LDQ

## 2.1 DQ localization in one dimension

The first step to localize DQ method is to find the neighborhood of a grid point of interest. We use

$$r_{il} = |x_i - x_l| \qquad i,l = 1,2,\ldots,N \tag{5}$$

to denote the distance between any two points in the solution domain. By comparison, we may find the permutation $s(1), s(2), \ldots, s(N)$ such that

$$r_{is(1)} \le r_{is(2)} \le \ldots \le r_{is(N)} \tag{6}$$

This is a typical permutation problem, and it is easy to find a suitable algorithm to solve the problem.

It is clear that the points falling in the neighborhood of $i$th point ($x_i$) are the first $m$ points which satisfy the above equation. Denote

$$S_i = (s(1), s(2), \ldots s(m)), \qquad i = 1,2,\ldots,N \tag{7}$$

and then $S_i$ defines the neighborhood of the grid point of interest. We may rewrite DQ approximation in this neighborhood in the form of

$$\frac{\mathrm{d}f(x_i,t)}{\mathrm{d}x} \approx \sum_{j \in S_i}^{N} a_{ij} f(x_j,t) \tag{8}$$

$$\frac{\mathrm{d}^2 f(x_i,t)}{\mathrm{d}x^2} \approx \sum_{j \in S_i}^{N} b_{ij} f(x_j,t) \tag{9}$$

Based on Quan and Chang (1989), the explicit formulae for the weighting coefficients are

$$a_{ij}(x) = \frac{1}{x_j - x_i} \prod_{\substack{k \in S_i \\ k \ne i,j}}^{N} \frac{x_j - x_k}{x_j - x_i} \qquad j \in S_i, j \ne i \tag{10}$$

$$a_{ii} = -\sum_{\substack{j \in S_i \\ j \ne i}}^{N} a_{ij} \tag{11}$$

$$b_{ij}(x) = 2(a_{ij}a_{ii} - \frac{a_{ij}}{x_i - x_j}) \qquad i,j = 1,\ldots,m, \qquad i \ne j \tag{12}$$

$$b_{ii}(x) = -\sum_{j \ne i}^{N} b_{ij}(x) \qquad i = 1,\ldots,m \tag{13}$$

## 2.2 Differential equation transformation

For applying LDQ to solve the problem, we can transform the above equation of the Sod shock tube problem into the following form:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial x} = -\frac{\partial q}{\partial x} \tag{14}$$

$$\frac{\partial q}{\partial t} = -\frac{\partial(qu)}{\partial x} - \frac{\partial p}{\partial x} = -\frac{\partial}{\partial x}(\frac{q^2}{\rho}) - \frac{\partial}{\partial x}\left[(\gamma - 1)(E - \frac{1}{2}\frac{q^2}{\rho})\right] \tag{15}$$

$$\frac{\partial E}{\partial t} = -\frac{\partial}{\partial x}\left[u(E+p)\right] = -\frac{\partial}{\partial x}\left\{\left[(\gamma - 1)(E - \frac{1}{2}\frac{q^2}{\rho}) + E\right]\frac{q}{\rho}\right\} \tag{16}$$

$$p = (\gamma - 1)(E - \frac{1}{2}\rho u^2) \tag{17}$$

Here we can define $q = \rho u$, for TNT explosive, $\gamma = 1.25$. Through the above transformation there are only three unknown variables $\rho$, $q$, $E$ to be calculated, meanwhile there exist three independent equations (Eqs.(14)–(16)), if the appropriate initial conditions are given. The above nonlinear ordinary differential equations can be solved by using any suitable numerical method.

In our program, the differential variables with regard to space variation can be calculated by using LDQ (such as $\partial q / \partial x$); the differential variables with regard to time variation (such as $\partial q / \partial t$) can be solved by using a fourth-order Runge-Kutta integrator.

# 3 Result and analysis

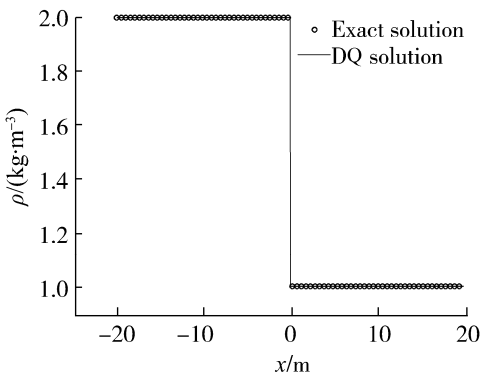
The whole program is written in FORTRAN language. Hereinafter, three examples are given to illustrate the problem and calculation results.

### 3.1 Example 1

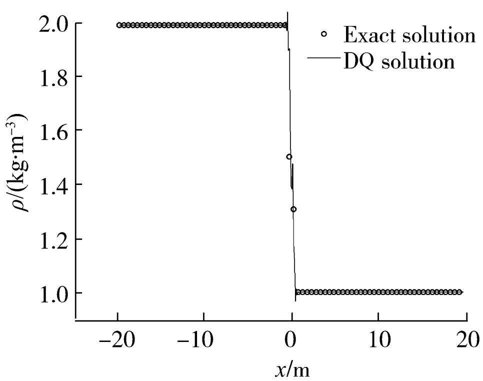
The initial conditions for this Sod shock tube problem can be given as:

$$(\rho,(\rho u),E)=\begin{cases}(2,0.0,3) & \text{if } x\le 0\\ (1,0,1.5) & \text{if } x>0\end{cases} \tag{18}$$

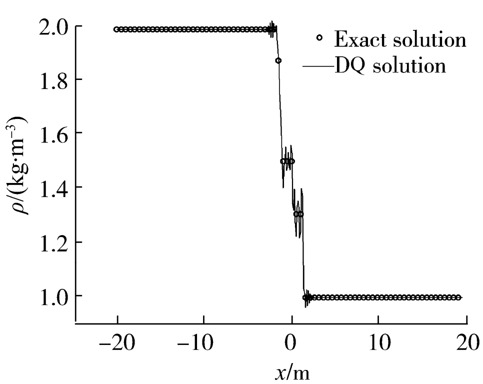
The calculation interval is from −20 m to 20 m and the number of calculation nodes are 400; the number of points falling in the neighborhood of *i*th point $x_i$ is *m*=5 (denoted by $m_{\rm set}$=5 in the program). The calculation time is 0–7.6 s, and the time step is 0.02 s. The evolutions of unknown variables $\rho$, $q$ and $E$ with time are shown in Fig.1, Fig.2 and Fig.3, respectively.



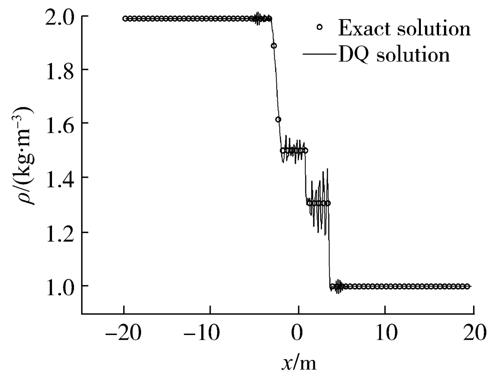
(a) *t*=0.0 s



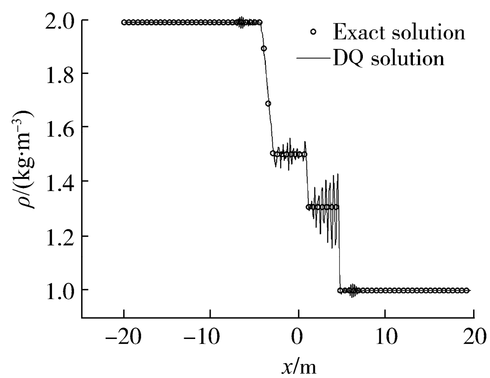
(b) *t*=0.4 s



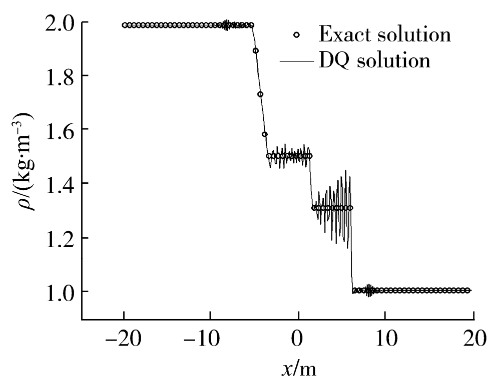
(c) *t*=2.0 s



(d) *t*=4.4 s

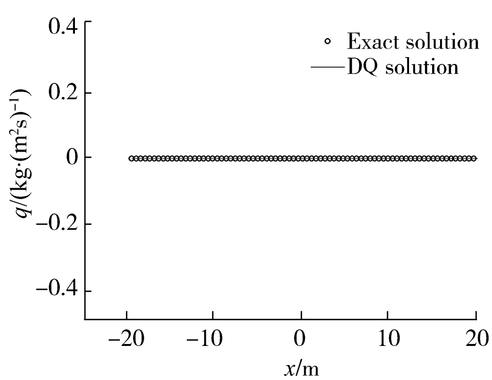


(e) *t*=6.0 s

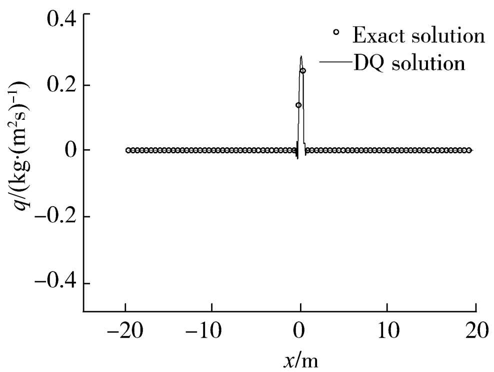


(f) *t*=7.6 s

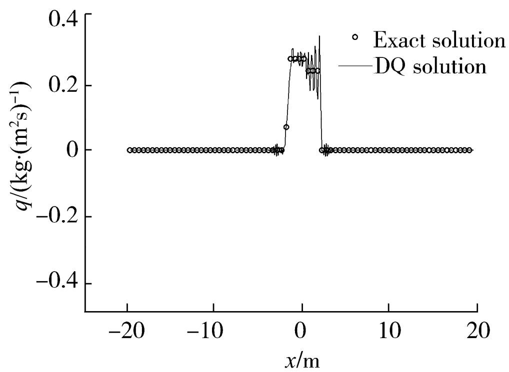
**Fig.1 Evolution of $\rho$ with time using LDQ**



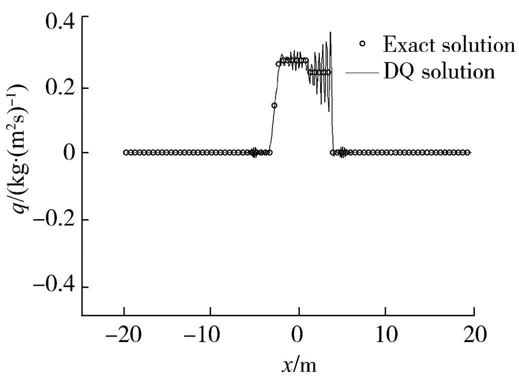
(a) *t*=0.0 s



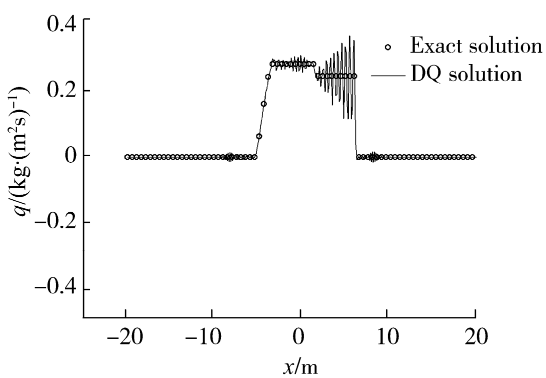
(b) $t$=0.4 s



(c) $t$=2.8 s

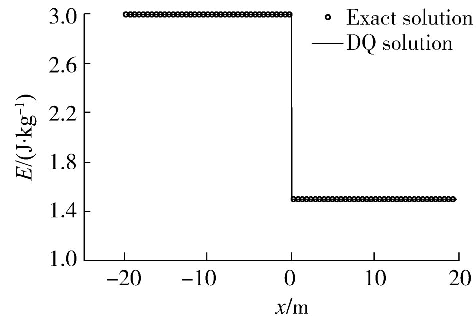


(d) $t$=4.8 s

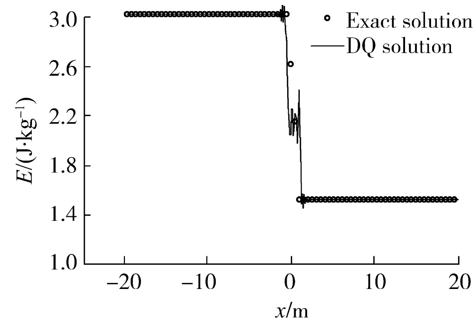


(e) $t$=7.6 s

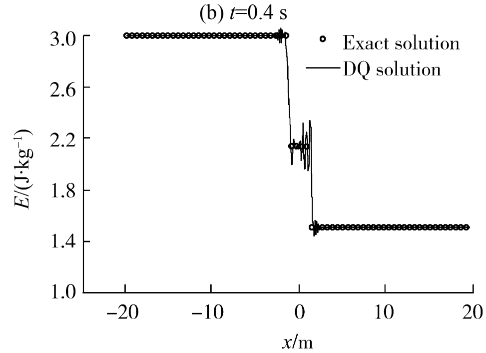
**Fig.2 Evolution of $q$ with time using LDQ**



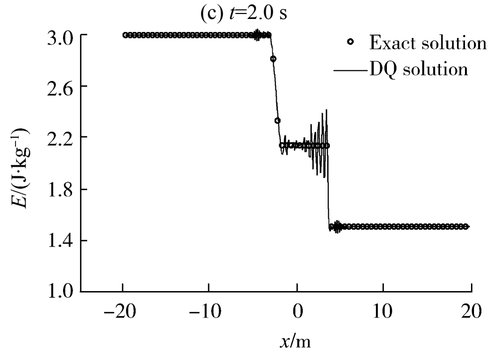
(a) $t$=0 s



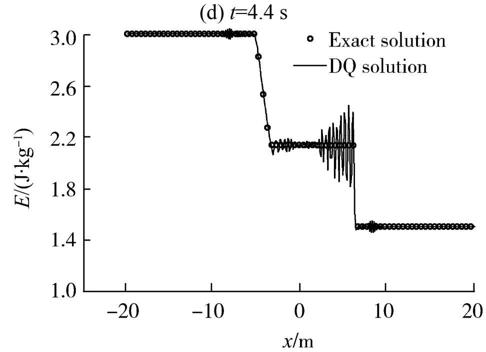
(b) $t$=0.4 s



(c) $t$=2.0 s



(d) $t$=4.4 s



(e) $t$=7.6 s

**Fig.3 Evolution of $E$ with time using LDQ**

Figs.1, 2 and 3 show the evolution of variable $\rho$, $q$, $E$ with time, respectively. As the figure shows, taking $\rho$ as an example, at time $t$=0.4 s, the values of $\rho$ in most parts are relatively smooth and stable except for some burrs appearing in the step point (that is $x$=0 m), as the time advances, the phenomenon of burrs is becoming more and more conspicuous. At time $t$=2 s, the serrated phenomenon has occurred in the vicinity of $x$=0 m, as the time goes by, it is aggravating obviously. Finally the calculation result has been completely deviated from the true value. The similar oscillation phenomenon also occurs to the other two variables $q$ and $E$.

**3.2 Example 2**

Another initial condition for this Sod shock tube problem can be given as shown in Fig.4.

The calculation interval is from −20 m to 20 m and the number of calculation nodes are 400; the number of points falling in the neighborhood of $i$th point $x_i$ is $m$=5 (denoted by $m_{set}$=5 in the program). The calculation time is 0–11.6 s, the time step is 0.02 s. The calculation result for the evolution of variable $\rho$ with time is shown in Fig.5.

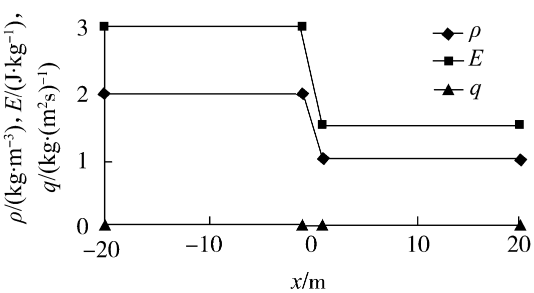
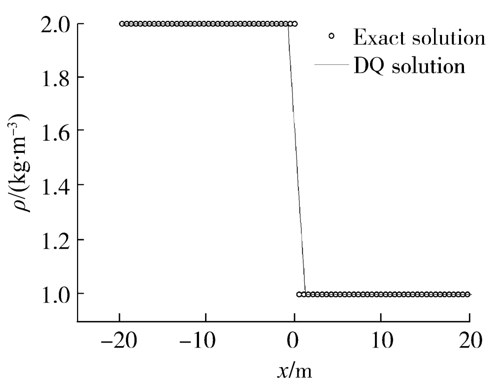
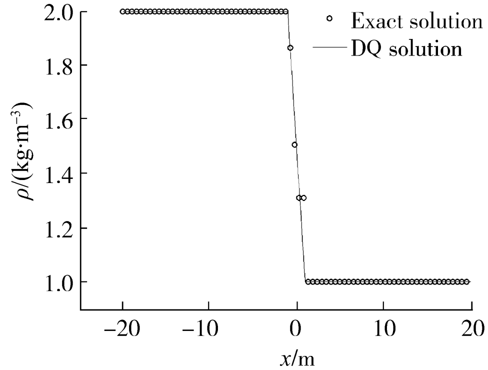


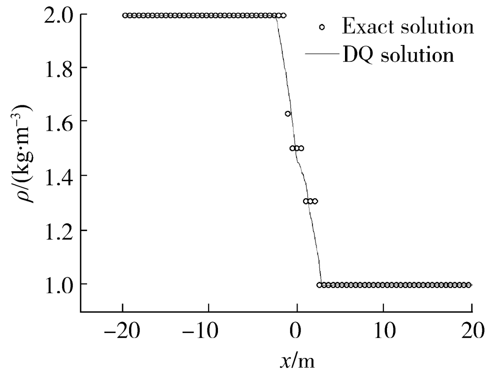

**Fig.4 Initial conditions for the Sod shock tube**



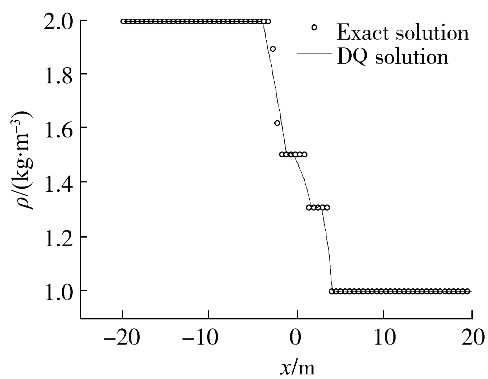

(a) $t$=0.0 s



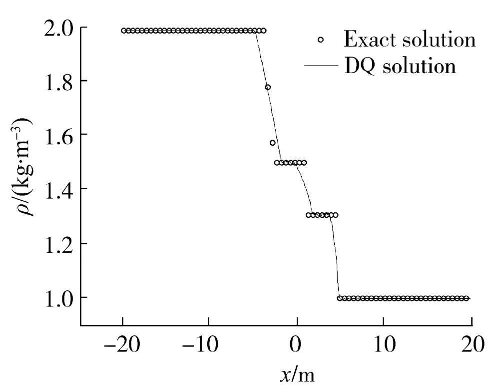

(b) $t$=1.2 s



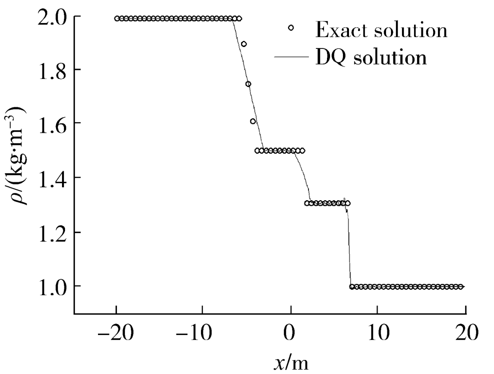

(c) $t$=2.4 s



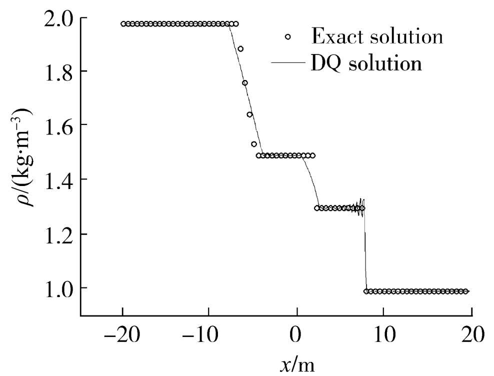

(d) $t$=4.4 s



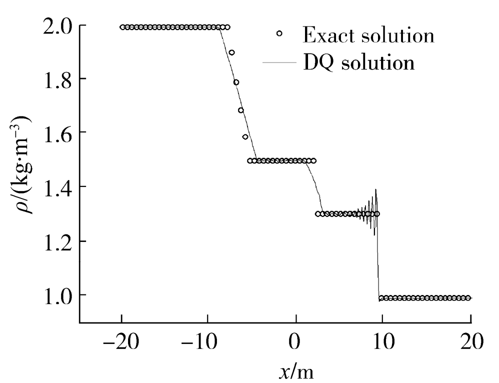

(e) $t$=5.6 s




(f) $t$=8.4 s




(g) $t$=10.2 s




(h) $t$=11.6 s

**Fig.5 Evolution of $\rho$ with time using LDQ**

The second initial condition given is less steep than the previous initial conditions at the step point (It is vertical at $x$=0 m in the example 1), the calculation results of $\rho$ are shown in Fig.5. In the beginning of the computation the wave form is relatively smooth, the whole LDQ solution matches well with the exact solution except that at the points of density discontinuity (Such as when $t$ = 2.4 s, the position in the vicinity of x=0 m). No obvious oscillations occur even when $t$=5.6 s. However, at time $t$=8.4 s the oscillations can be observed at the position in the neighborhood of $x$=8 m. At time $t$=10.2 s and $t$=11.6 s, the oscillations become very obvious. In conclusion, the calculation result tends to divergence in the end; however, compared with the oscillations in the example 1, the amplitude and occurring time of oscillations have been improved a lot in the example 2.

### 3.3 Example 3

In the third case, the original equations are corrected by adding one term $\varepsilon\frac{\partial^2 q}{\partial x^2}$ to the right side of Eq.(15), and then we can obtain:

$$\frac{\partial \rho}{\partial t}=-\frac{\partial(\rho u)}{\partial x}=-\frac{\partial q}{\partial x} \tag{19}$$

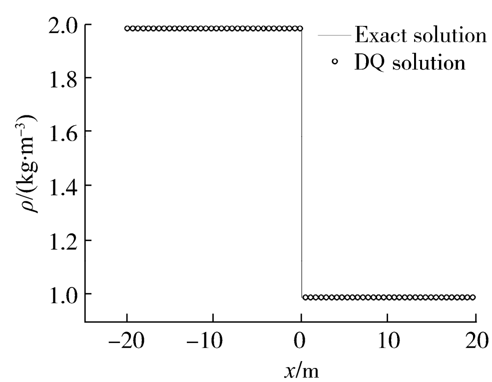
$$\frac{\partial q}{\partial t}=-\frac{\partial(qu)}{\partial x}-\frac{\partial p}{\partial x}=-\frac{\partial}{\partial x}\left(\frac{q^2}{\rho}\right)-\frac{\partial}{\partial x}\left[(\gamma-1)\left(E-\frac{1}{2}\frac{q^2}{\rho}\right)\right]+\varepsilon\frac{\partial^2 q}{\partial x^2} \tag{20}$$

$$\frac{\partial E}{\partial t}=-\frac{\partial}{\partial x}\left[u(E+p)\right]=-\frac{\partial}{\partial x}\left\{\left[(\gamma-1)\left(E-\frac{1}{2}\frac{q^2}{\rho}\right)+E\right]\frac{q}{\rho}\right\} \tag{21}$$

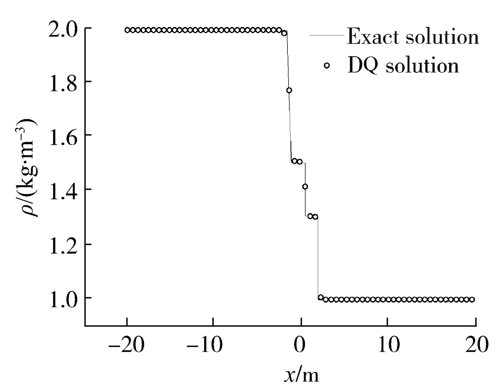
$$p=(\gamma-1)\left(E-\frac{1}{2}\rho u^2\right) \tag{22}$$

$$q=\rho u \tag{23}$$

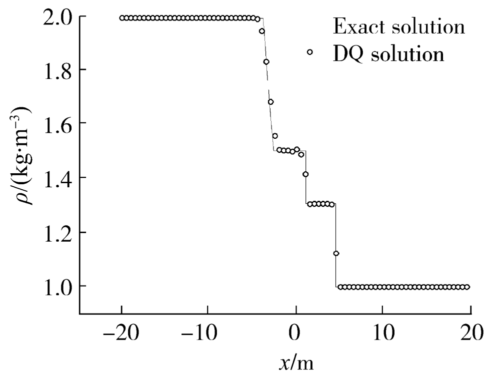
where $\varepsilon = 0.02$, the time step is 0.01 s; other conditions are the same to those given in the example 1. The results of $\rho$ can be obtained and plotted in Fig.6.



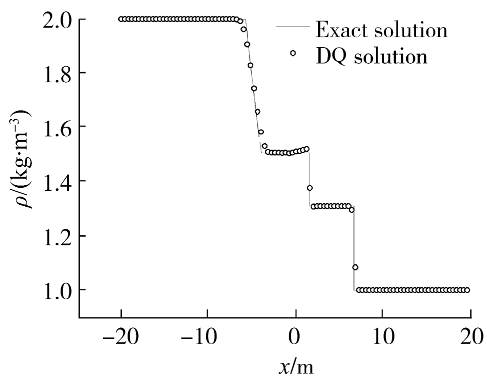

(a) $t$=0.0 s



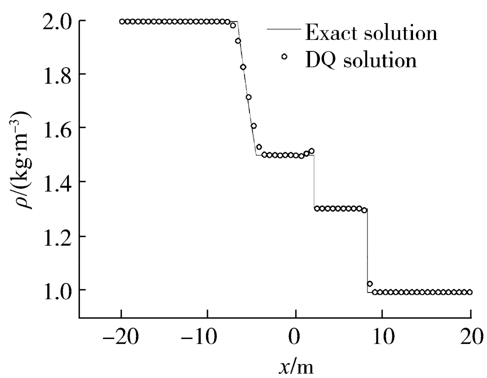

(b) $t$=2.4 s



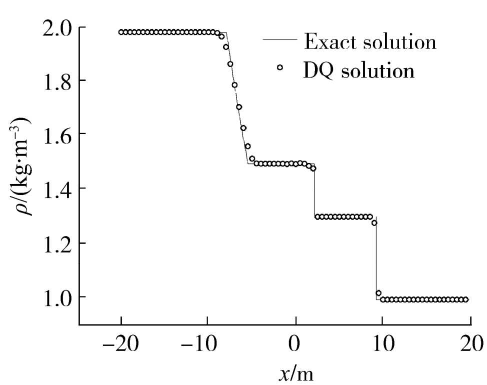

(c) $t$=5.6 s



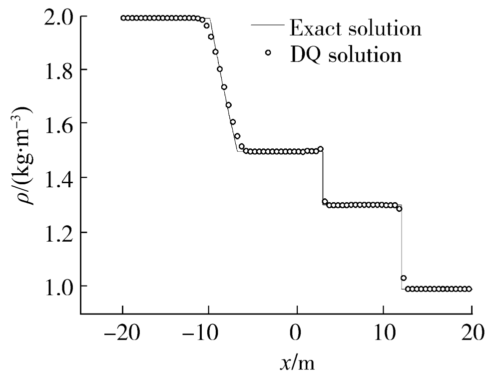

(d) $t$=8.4 s




(e) $t$=10.0 s




(f) $t$=11.6 s




(g) $t$=14.8 s

**Fig.6 Evolution of $\rho$ with time using LDQ**

The evolution of $\rho$ with time is very stable in the whole process of calculation. Only some slight oscillations appear in the vicinity of $x$=0 m at $t$=5.6 s, but the oscillations gradually reduce and disappear as the time goes by. At $t$=11.6 s, the LDQ solution is much more accurate and robust in the example 3 than that in the example 2. (Very fierce oscillations can be observed in the example 2). Even at $t$=14.8 s, the LDQ solution is still very stable and not any conspicuous oscillation occur to any parts of the solution position.

So by adding appropriate artificial viscosity at the momentum equation, we can eliminate the serrated wave form effectively when using the LDQ. The numerical solution is very smooth and stable. The disappearance of oscillations can also be found for other two variables $q$ and $E$ compared with those in the first example. From the figure given above, the LDQ solution is in very good agreement with the exact solution.

## 4 Conclusions

LDQ is a numerical technique of high accuracy. This method is accurate and effective for most of the problems. However, in this paper it reveals some difficulties by directly applying LDQ scheme to solve some very particular problems. In LDQ, the computation of the derivatives at $x_i$ is to use the weighted sum of the function values of the neighboring points. It is reasonable for the smooth and continuous functions; however, it may be irrational for the step functions or discontinuous functions. Most of finite difference schemes assume that the solution is smooth, i.e., the derivatives are bounded, so that a Taylor series expansion in the spatial step size $\Delta x = x_{i+1} - x_i$ is valid. When this assumption is violated by a discontinuity, a first order scheme tends to smear out the discontinuity, including higher orders results in unstable oscillations of the solution at the position of the discontinuity. For such kind of problems, it is more reasonable to calculate derivatives of step function by adopting some corrections.

In the first example, we obtained the results of the Sod shock tube problem by directly applying the LDQ Scheme, very serious numerical oscillations could be observed in the process of calculation. The solution of the problem tended to diverge from the exact solution in the end. In the second example, some adjustments were made to the initial conditions of the Sod shock tube problem; although some numerical oscillations still could be found in the final phase, the serrated wave forms were mitigated sharply compared to those in the first example. In the third example, the numerical oscillations almost vanished by adding artificial viscosity in the momentum equation of the Sod shock tube problem. It was very stable and robust for the whole process of calculation, and the numerical solution was very close to the exact solution.

From solving the Sod shock tube problem, we can know that LDQ may meet some difficulties in solving some very particular problems, the numerical solutions may not be very ideal than that we expect or even wrong. Solving this kind of particular problems should be treated specially. In Sod shock tube problem, strong numerical oscillations occurred when LDQ was directly applied to solve the problem, but the oscillation phenomenon could be efficiently reduced or even eliminated when proper initial values were given or the artificial viscosity was added to momentum the equation. However, in general, it is very clear that LDQ is highly accurate and effective for solving most of nonlinear problems.

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**Zhi Zong** was born in 1964. He is a professor of Dalian University of Technology. His current research interests include: 1) computational mechanics and computational methods (FEM, BEM, differential quadrature, meshless method, SPH, VOF); 2) Linear and non-linear dynamics (solid mechanics, fluid mechanics, shock, impact, sound and vibration); 3) fluid-structure interactions in engineering and in the human body, *etc*.

**Zhangrui Li** was born in 1985. He is a phD candidate of the Department of Naval Architecture and Ocean Engineering at Dalian University of Technology. His current research field includes: numerical calculation, bubble dynamics of underwater explosion and the response of the ship subjected to the underwater explosion loading.

**Jing Dong** was born in 1986. She is a master student of the Department of Naval Architecture and Ocean Engineering at Dalian University of Technology. Her current research field is numerical simulation of the vortex induced vibration of the deep ocean riser using discrete vortex method.