Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Journal of Computational Physics 202 (2005) 699–709
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

On criterions for smoothed particle hydrodynamics kernels in stable field

Jin Hongbin, Ding Xin *

College of Textiles, Donghua University, 1882 West Yan-an Road, Shanghai 200051, PR China

Received 3 December 2003; received in revised form 5 August 2004; accepted 5 August 2004
Available online 11 September 2004

Abstract

Smoothed particle hydrodynamics (SPH) particle approximation equations for functions and their derivatives are analyzed in stable field. Three criterions for determining suitable kernels are proposed to evaluate the accuracy of computation. The first criterion is used to evaluate the estimation errors of the functions. The second and third criterions are for the first derivatives of the functions. The second criterion requires that the first derivative of a kernel should be zero when the position of the neighbor particle is approaching the estimated one. The third criterion is so defined that the particle estimation of the first derivatives in stable field should be zero. Ten SPH kernels with different orders of function are selected to demonstrate the application of the criterions. The effects of the position of the estimated particles and the smoothing length on behaviors of the kernels are analyzed. To verify the feasibility of the three criterions in dynamic field, one dimensional shock tube problem is simulated with four deliberately chosen kernels. The simulation results, including profiles of density, pressure, velocity and energy, are compared with the exact solutions. Through analyses, it is found that the three criterions proposed in this study are feasible to evaluate the properties of kernels. Of the three criterions, the first one is more critical than the other two. In terms of computational accuracy, Gaussian and Q-spline kernels can be regarded as the best kernels of the ten proposed kernels in this study.

Keywords: Kernels; Smoothed particle hydrodynamics; Criterion

1. Introduction

The foundation of smoothed particle hydrodynamics (SPH) is the interpolation theory [3,7,9]. Using a suitable interpolation kernel is therefore the basic requirement for correct computational results. A suitable kernel must have two properties as suggested by Monaghan and coworker [3,9]

* Corresponding author. Tel.: +862162373651.
E-mail addresses: jhb@mail.dhu.edu.cn (J. Hongbin), xding@dhu.edu.cn (D. Xin).

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2004.08.002

$$\int_{\Omega} W(x - x', h)\,\mathrm{d}x' = 1 \tag{1}$$

and, when the smoothing length $h \to 0$ the kernel can be approximated by the Dirac delta function

$$\lim_{h\to 0} W(x, h) = \delta(x). \tag{2}$$

Monaghan [10] also suggests that a suitable kernel must have a compact support in order to ensure zero interactions outside its computational range. Take the Gaussian kernel [3] as an example. Although it meets the basic conditions presented by Eqs. (1) and (2), it does not meet the requirement of a compact support so that the computational efficiency is rather low. Various kernels with a compact support have been established, such as super Gaussian kernel [11], spline kernels [8], polynomial kernels [4] and cosine kernel [2]. The computational range of these kernels is usually no more than three times the smoothing length.

Recent studies [10,12] indicate that the stability of the SPH algorithm depends strongly upon the second derivative of the kernels. For example, the second derivative of lower-order spline kernels is a piecewise-linear function, and accordingly, the stability is inferior to those of higher-order kernels. Therefore, higher-order spline kernels are used more frequently, especially in simulating the flow behavior of quasi-incompressible fluids [1,12].

A kernel must be accurate to minimize the errors caused by using the interpolation method. Monaghan [10] analyzes the estimation errors of the method and states that the errors are proportional to h^2 when the kernel is an even function of x, or to h^4 when the kernel satisfies the following equation:

$$\int x^2 W(x, h)\,\mathrm{d}x = 0. \tag{3}$$

As a matter of fact, not all of the suitable kernels meet this requirement [2]. Roberto and Roberto [13] suggest an additional criterion for selecting suitable kernels, i.e., any accurate kernels must meet the requirement of minimizing the estimation errors to the derivative of a given function. They take two kernel functions, the third-order spline and the super-Gaussian, as examples to demonstrate the application of the criterion.

In fact, the errors of SPH method come from two sources: kernel approximation and particle approximation. As a result, even if Eq. (3) is satisfied, the estimation results by SPH method could not be accurate. Fulk and Quinn [2] analyze the errors from the particle approximation of first derivatives and give a criterion with the summation form for evaluating the kernels. Twenty different kernels are analyzed and the bell shaped kernels show better performance than other ones.

In this study the particle approximation equations for functions and their derivatives are applied in a stable field. Concentrated on the accuracy of computation, three criterions for determining suitable kernels are proposed. Ten SPH kernels are used to demonstrate the use of the criterions. Furthermore, a shock tube problem is simulated with four deliberately chosen kernels to verify the feasibility of the proposed criterions.

2. Criterions from the interpolation equation of the function

The basic form of the SPH interpolation equation [10]

$$\langle f_i \rangle = \sum_j \frac{m_j}{\rho_j} f_j W_{ij}. \tag{4}$$

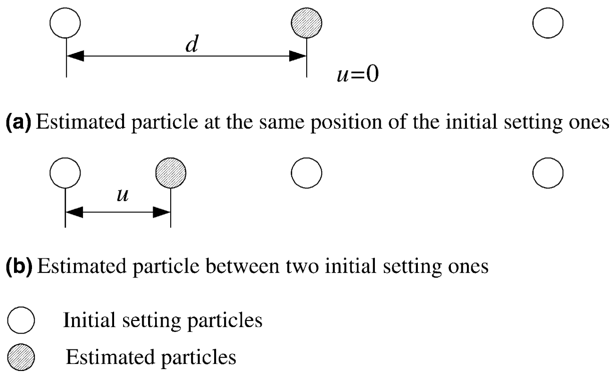

Fig. 1. Position of an estimated particle and initial setting ones.

In Eq. (4), subscript j denotes the initial setting particles, of which the variables are known. Subscript i represents the estimated particles. For convenient reason, the estimated particles can either be the initial setting particles or the particles between the initial setting ones. In the latter case, the estimated particles are actually not true particles but those in different positions from the initial setting ones, of which the variables can also be estimated by the initial setting particles. The relationship between the initial setting particles and an estimated one is illustrated in Fig. 1.

In a stable field where the variables are independent of the spatial position, e.g. $f_i = f_j$, $\rho_i = \rho_j$, $m_i = m_j$, Eq. (4) can be rewritten as

$$d^{\lambda}\sum_j W_{ij} = d^{\lambda} \times \left(W\left(\frac{u}{\alpha d}\right) + W\left(\frac{1}{\alpha} - \frac{u}{\alpha d}\right) + W\left(\frac{1}{\alpha} + \frac{u}{\alpha d}\right) + W\left(\frac{2}{\alpha} - \frac{u}{\alpha d}\right) + \cdots\right) = 1, \tag{5}$$

where $d^{\lambda} = m/\rho$, λ (=1, 2 or 3) is the number of dimensions, u ($0 \leqslant u \leqslant d/2$) is the distance between the estimated particle and the nearest initial setting one, α ($0.8 \leqslant \alpha = h/d \leqslant 1.5$, usually $\alpha = 1$) is the smoothing length in dimensionless form [5].

By definition

$$M\left(\frac{u}{d},\alpha\right) = d^{\lambda} \times \left(W\left(\frac{u}{\alpha d}\right) + W\left(\frac{1}{\alpha} - \frac{u}{\alpha d}\right) + W\left(\frac{1}{\alpha} + \frac{u}{\alpha d}\right) + W\left(\frac{2}{\alpha} - \frac{u}{\alpha d}\right) + \cdots\right).$$

Eq. (5) becomes

$$M\left(\frac{u}{d},\alpha\right) = 1. \tag{6}$$

Eq. (6) is regarded as the first criterion for all suitable kernels. Only when a kernel satisfies the first criterion could it give correct estimation results of the function.

3. Criterions from the interpolation equation of the derivative

The basic form of SPH interpolation equation of the first derivative [10] shows

$$\langle f' \rangle = \sum_j \frac{m_j}{\rho_j} f_j W_{ij,x}, \tag{7}$$

where $W_{ij,x} = \frac{\partial W}{\partial x} = \frac{\partial W}{\partial r}\frac{\mathrm{d}r}{\mathrm{d}x}$ and $\frac{\mathrm{d}r}{\mathrm{d}x} = \frac{\mathrm{d}(|x|/h)}{\mathrm{d}x} = \frac{x}{h|x|}$. Eq. (7) indicates that the first derivative of the function could be approximated by the values of the function at the initial setting particles and the first derivative of the kernel.

When $x \to 0$, i.e., $r \to 0$, $\lim_{x\to 0^-} \frac{x}{|x|} = -1$ and $\lim_{x\to 0^+} \frac{x}{|x|} = +1$. Because $\lim_{x\to 0^-} \frac{x}{|x|} \neq \lim_{x\to 0^+} \frac{x}{|x|}$, $\lim_{x\to 0} \frac{\mathrm{d}r}{\mathrm{d}x}$ is inexistent. However, Eq. (7) can still be used should the kernels meet the following criterion:

$$\left.\frac{\partial W}{\partial r}\right|_{r=0} = 0. \tag{8}$$

Eq. (8) is regarded as the second criterion for suitable kernels.

When Eq. (7) is used in a stable field, it becomes

$$fd^{\lambda} \sum W_{ij,x} = fd^{\lambda} \sum \frac{\partial W_{ij}}{\partial r}\frac{\mathrm{d}r}{\mathrm{d}x} = fd^{\lambda}\frac{1}{h}\sum \frac{\partial W}{\partial r}\frac{x}{|x|} = 0. \tag{9}$$

By definition

$$N\left(\frac{u}{d},\alpha\right) = \sum \frac{\partial W}{\partial r}\frac{x}{|x|} = \frac{\partial W}{\partial r}\left(\frac{u}{\alpha d}\right) - \frac{\partial W}{\partial r}\left(\frac{1}{\alpha} - \frac{u}{\alpha d}\right) + \frac{\partial W}{\partial r}\left(\frac{1}{\alpha} + \frac{u}{\alpha d}\right) - \frac{\partial W}{\partial r}\left(\frac{2}{\alpha} - \frac{u}{\alpha d}\right) + \cdots$$

Eq. (9) becomes

$$N\left(\frac{u}{d},\alpha\right) = 0. \tag{10}$$

Eq. (10) is chosen as the third criterion for suitable kernels. Only when a kernel satisfies the third criterion could it give correct estimation results of the first derivative of a function.

From the definition of N, it is understood that Eq. (10) is always satisfied when $u = d/2$. In addition, when $u = 0$, Eqs. (10) and (8) are identical. In other words, the second criterion is a special case of the third one when $u = 0$.

4. Analysis of select kernels

Of the three criterions, the second one is easier to use than the other two. Therefore, to evaluate the suitability of a chosen kernel it is suggested to check the kernel first with the second criterion.

To demonstrate the application of the three criterions proposed in this study, 10 kernels in one dimension are selected and listed in Table 1. Some of the kernels are directly from published literature and others are proposed here for the first time.

First, the second criterion is used to evaluate the suitability of the kernels. By Eq. (8) values of $\partial W/\partial r(0)$ are calculated and shown in Table 1. It can be seen that all of the kernels satisfy the condition of the second criterion except Quadric 1 and '1/X, 2' kernel. These two kernels are considered unsuitable for the estimation of the first derivatives and may not require further evaluation by other two criterions.

Then, the first and third criterions are put forward. From Eqs. (6) and (10) it is known that the values of M and N depend on two variables, the position of the estimated particle u/d and the dimensionless smoothing length α. Figs. 2 and 3 show, respectively, the variations of M and N with the position of the estimated particle for the proposed kernels. It can be seen that the values of M and N depend on the position of the estimated particle, u/d, except Gaussian and Q-spline kernels, which can always satisfy the first and the third criterions wherever the estimated particle locates. It can also be seen that Quadric 2 kernel might

Table 1
Select kernels together with the results by the second criterion

No.	Name	Expression	$\partial W/\partial r(0)$
1	Gaussian	$\frac{1}{\sqrt{\pi}h}e^{-r^2}$	0
2	B-spline	$\frac{1}{h}\begin{cases} 2/3 - r^2 + 0.5r^3, & 0\leqslant r<1,\\ (2-r)^3/6, & 1\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	0
3	Double B-spline	$\frac{1}{h}\begin{cases} 2r^2 - 3r^4 + 1.5r^5, & 0\leqslant r<1,\\ r^2(2-r)^3/2, & 1\leqslant r<2,\\ 0, & r\geqslant 2,\end{cases}$	0
4	Q-spline	$\frac{1}{120h}\begin{cases} (3-r)^5 - 6(2-r)^5 + 15(1-r)^5, & 0\leqslant r<1,\\ (3-r)^5 - 6(2-r)^5, & 1\leqslant r<2,\\ (3-r)^5, & 2\leqslant r<3,\\ 0, & r\geqslant 3.\end{cases}$	0
5	Quadric 1	$\frac{1}{h}\begin{cases} 3(2-r)^2/16, & 0\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	−0.75
6	Quadric 2	$\frac{1}{h}\begin{cases} 3(4-r^2)/32, & 0\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	0
7	Thrice	$\frac{1}{h}\begin{cases} (2-r)^2(r+1)/8, & 0\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	0
8	Quartic	$\frac{1}{h}\begin{cases} 5(2-r)^3(3r+2)/128, & 0\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	0
9	Cosine	$\frac{1}{h}\begin{cases} \frac{3\pi^2}{8(\pi^2+3)}(1-\frac{r^2}{4})(1+\cos(\frac{\pi r}{2})), & 0\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	0
10	1/X, 2	$\frac{1}{h}\begin{cases} \frac{1}{\ln 4 - 1.25}(\frac{1}{2+r}+\frac{r-6}{16}), & 0\leqslant r<2,\\ 0, & r\geqslant 2.\end{cases}$	−1.38

not be a suitable kernel because the values of M and N are far more away from the desired values than other kernels. Furthermore, the worst results of M can always be found when $u = 0$ or $u = d/2$ and the worst results of N are somewhere between $u = 0$ and $u = d/2$.

In addition to the effects of the estimated particle position, Figs. 4 and 5 illustrate the effects of the smoothing length. To improve the accuracy of SPH computation, the number of neighbor particles of one particle should remain constant. To meet this requirement the smoothing length should be a variable during the entire simulation process [7]. This requirement will lead to the low efficiency of SPH method.

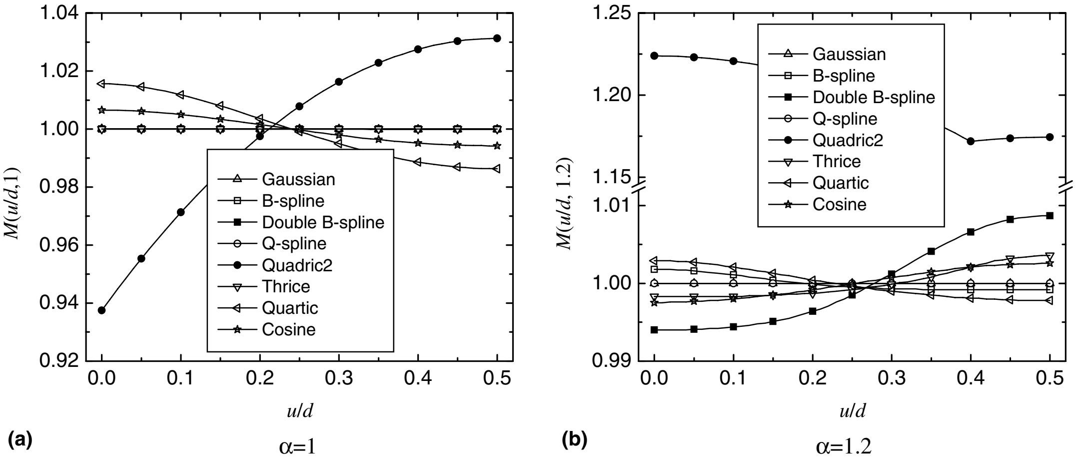

Fig. 2. Influence of the estimated particle position on M.

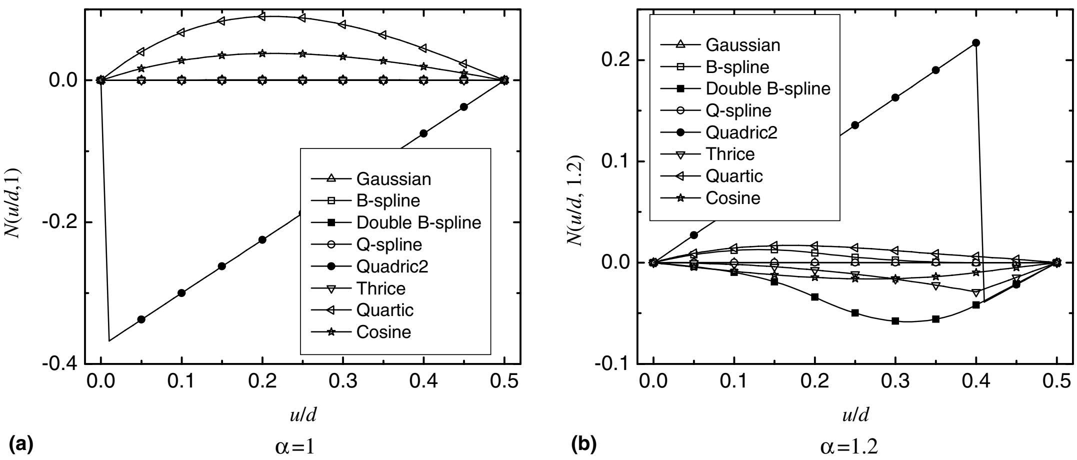

Fig. 3. Influence of the estimated particle position on N.

Therefore, it is desirable that the values of M and N should not be too sensitive to the smoothing length in order to avoid the scheme of change the smoothing length. From this point of view, Quadric 2 and double B-spline kernels might not be considered as suitable kernels. On the other hand, the values of M and N for Gaussian and Q-spline kernels seem to be independent of the smoothing length.

To evaluate the performance of kernels quantitatively, following equations are used to calculate the deviation of M and N of the proposed kernels from the desired values by Eqs. (6) and (10):

$$l_1 = \sqrt{\frac{1}{m} \times \frac{1}{n} \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} (M(i\delta, j\delta + \alpha_0) - 1)^2}, \tag{11}$$

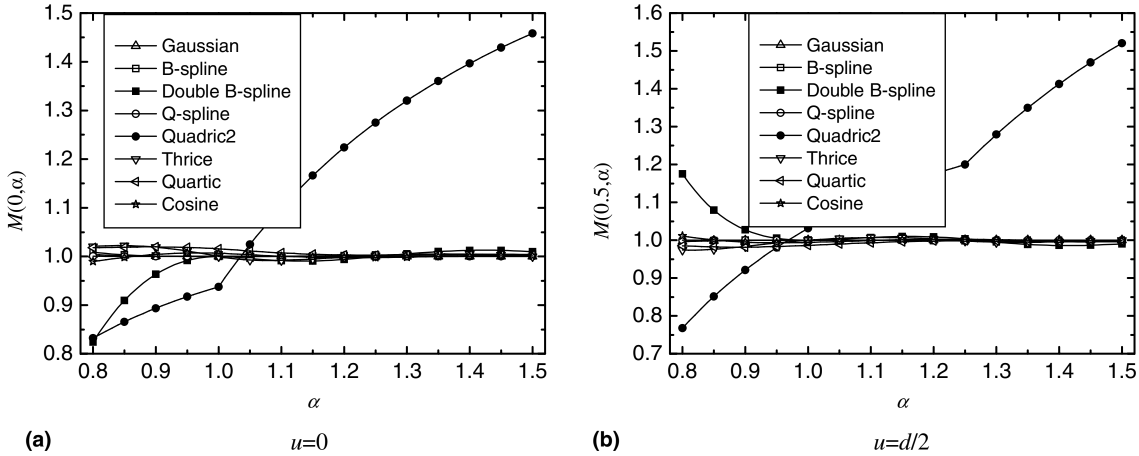

Fig. 4. Influence of the smoothing length on M.

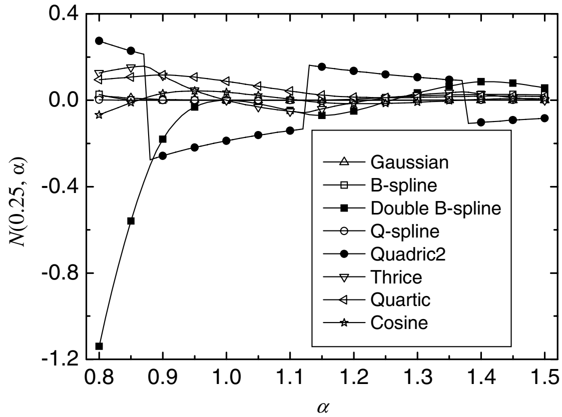

Fig. 5. Influence of the smoothing length on N.

$$l_2 = \sqrt{\frac{1}{m} \times \frac{1}{n} \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} \left(N(i\delta, j\delta + \alpha_0)\right)^2}, \tag{12}$$

where l_1 and l_2 are the mean square deviation of $(M - 1)$ and N, respectively. δ is the interval of u/d and α. m and n are the number of data of u/d and α, respectively, within the domain, i.e., $u/d \in [0.0,0.5]$ and $\alpha \in [0.8,1.5]$. α_0 is the minimum value of α.

Fig. 6 is a bar chart showing the deviations of 10 kernels calculated by Eqs. (11) and (12). Results of l_1 show that Quadric 2 (No. 6) is the least favorite kernel. While from the values of l_2 Quadric 1 (No. 5) and '1/X, 2' (No. 10) are certainly not good kernels, neither double B-spline (No. 3) nor Quadric 2 (No. 6). From both results of l_1 and l_2 a summation can be made that the most suitable kernels are Gaussian (No. 1) and

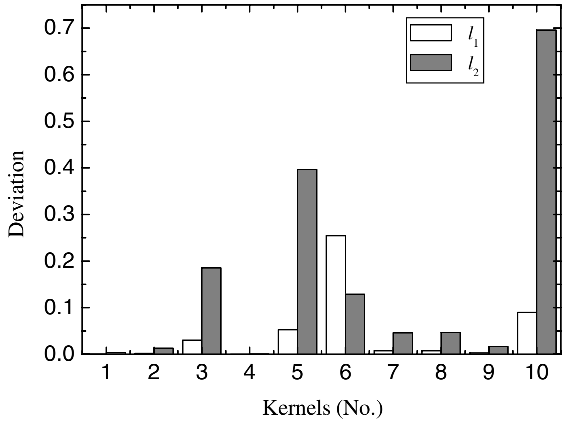

Fig. 6. Bar chart of the evaluation results.

Q-spline (No. 4), which can best meet the requirements of the three criterions proposed in this study. It also shows that the lower the order of kernel is, the larger the values of l_1 and l_2 are. The values of l_1 and l_2 for Quadric kernels (No. 5 and No. 6) are distinctly larger than those of Thrice, Quartic, B-spline and Q-spline kernels due to the lower-order approximation of the former to the first derivative. This is the reason why higher-order kernels exhibit superior stability in SPH simulations where evaluations of the first- and second-order derivatives are required.

5. A numerical test

To verify the feasibility of the three criterions, the shock tube problem, which is a good numerical benchmark and used by many researchers when studying SPH [6,11], is simulated by SPH method with four kernels. They are Q-spline, which meets the requirements of the three criterions, Quadric 1, of which $\partial W/\partial r(0) \neq 0$, Quadric 2, of which $\partial W/\partial r(0) = 0$ but the value of l_1 is the largest, and Quartic, of which $\partial W/\partial r(0) = 0$ but the value of l_2 is lower than that of Quadric 2.

The initial conditions of the shock tube are similar to what Hernquist and Katz [6] used, i.e.:

$$x \leqslant 0, \quad \rho = 1, \quad v = 0, \quad e = 2.5, \quad p = 1, \quad d = 0.001875,$$

$$x > 0, \quad \rho = 0.25, \quad v = 0, \quad e = 1.795, \quad p = 0.1795, \quad d = 0.0075,$$

where ρ, p, e and v are the density, pressure, internal energy and velocity of the gas, respectively, d is the distance between the initial setting particles.

There are 400 particles used in the simulation. 320 particles are evenly distributed in the high-density region [−0.6 to 0.0] and 80 particles in the low-density region [0.0 to 0.6]. All particles have the same mass of 0.001875. The smoothing length is taken as 0.015. The equation of state for the ideal gas, $p = (\gamma - 1)\rho e$, is used in the simulation with $\gamma = 1.4$. The time step is 0.003 and the simulation runs for 50 time steps. The SPH equations used are as follows:

$$\rho_i = \sum_j m_j W_{ij}, \tag{13}$$

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = -\sum_j m_j \left(\frac{\sigma_i}{\rho_i^2} + \frac{\sigma_j}{\rho_j^2} + \Pi_{ij} \right) W_{ij,x}, \tag{14}$$

$$\frac{\mathrm{d}e_i}{\mathrm{d}t} = \frac{1}{2} \sum_j m_j (v_i - v_j) \left(\frac{\sigma_i}{\rho_i^2} + \frac{\sigma_j}{\rho_j^2} + \Pi_{ij} \right) W_{ij,x}, \tag{15}$$

where m is the mass, v is the velocity, σ is the stress, Π is the artificial viscosity, which is used to prevent unphysical oscillations near shocks [10].

Fig. 7 shows the density, pressure, velocity and internal energy profiles. It can be seen that the obtained results by Q-spline and Quartic kernels agree well with the exact solution in the region [−0.4 to 0.4]. The shock is observed from $x = 0.2$–0.25. The rarefaction wave is located between $x = -0.2$ and 0. However, the estimation density and pressure in front of the shock by Quadric 1 seem to be slight larger than the exact solution because the kernel does not satisfy the second criterion. As to Quadric 2 kernel, estimation results are unstable and far away from the exact solutions as shown in Fig. 7. This is caused by the fact that the

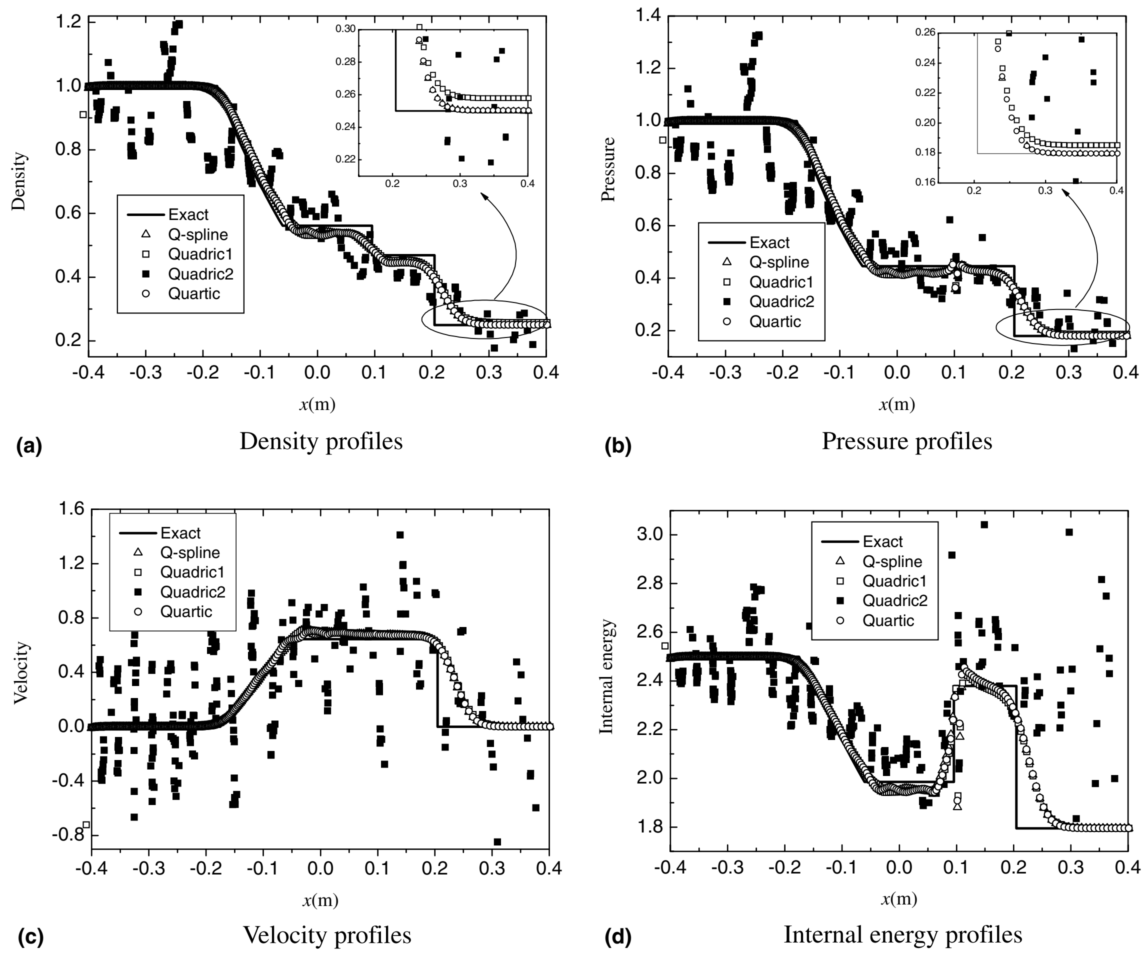

Fig. 7. Simulation results for the shock tube at $t = 0.15$ s.

value of l_1 for the kernel is the largest among the proposed kernels. Therefore, the estimation error of the density is quite noticeable. As a matter of fact, an accurate estimation of density by SPH method is the most important process because density appears in almost all of the SPH interpolation equations, e.g. Eqs. (14) and (15). From this point of view, the first criterion is more critical than the other two.

The numerical test demonstrates that, although the three criterions are developed from the analysis of SPH equations in the stable field, the properties of kernels evaluating by them are in accordance with the application in dynamic field.

6. Conclusions

In this study the particle approximation equations for functions and their derivatives are applied in the stable field. Three criterions are proposed for evaluating the computational accuracy of SPH kernels. Ten SPH kernels are used to demonstrate the application of the criterions. In addition, one dimensional shock tube problem is simulated with four deliberately chosen kernels to verify the feasibility of the proposed criterions.

The following conclusions can be made:

1. Three criterions are developed for evaluating suitable kernels. The first criterion is used to evaluate the estimation errors of the function, while the other two are for those of the first derivative.
2. Of the three criterions, the first criterion is more critical than the other two.
3. In terms of computational accuracy, Gaussian and Q-spline kernels can be regarded as the best kernels of 10 proposed kernels in this study. However, Quadric 1, Quadric 2 and '1/X, 2' kernels can be considered as the least favorite ones.

Acknowledgements

The authors express their sincere thanks to the two anonymous reviewers for their very valuable comments and suggestions, which greatly improved the quality of this paper.

References

[1] J.K. Chen, A generalized smoothed particle hydrodynamics method for nonlinear dynamic problems, Comput. Meth. Appl. Mech. Eng. 190 (2000) 225–239.
[2] D.A. Fulk, D.W. Quinn, An analysis of 1-D smoothed particle hydrodynamics kernels, J. Comput. Phys. 126 (1996) 165–180.
[3] R.A. Gingold, J.J. Monaghan, Smoothed particle hydrodynamics: theory and application to non-spherical stars, Mon. Not. R. Soc. 181 (1977) 375–389.
[4] R.A. Gingold, J.J. Monaghan, Kernel estimates as a basis for general particle methods in hydrodynamics, J. Comput. Phys. 46 (1982) 429–453.
[5] R.J. Gordon, A.S. Robert, R.B. Stephen, SPH for high velocity impact computations, Comput. Meth. Appl. Mech. Eng. 139 (1996) 347–373.
[6] L. Hernquist, N. Katz, TreeSPH: a unification of SPH with the hierarchical tree method, Astrophys. J. Suppl. Ser. 70 (1989) 419–446.
[7] L.D. Libersky, A.G. Petschek, T.C. Carney, J.R. Hipp, F.A. Allahdadi, A high strain Lagrangian hydrodynamics, J. Comput. Phys. 109 (1993) 67–75.
[8] J.J. Monaghan, Extrapolating B-splines for interpolation, J. Comput. Phys. 60 (2) (1985) 253–262.
[9] J.J. Monaghan, An introduction to SPH, Comput. Phys. Commun. 48 (1988) 89–96.
[10] J.J. Monaghan, Smoothed particle hydrodynamics, Ann. Rev. Astron. Astrophys. 30 (1992) 543–574.

[11] J.J. Monaghan, R.A. Gingold, Shock simulation by the particle method SPH, J. Comput. Phys. 52 (1983) 374–389.
[12] J.P. Morris, P.J. Fox, Y. Zhu, Modeling low Reynolds number incompressible flows using SPH, J. Comput. Phys. 136 (1997) 214–226.
[13] C.D. Roberto, D.L. Roberto, A criterion for the choice of the interpolation kernel in smoothed particle hydrodynamics, Appl. Numer. Math. 34 (2000) 363–371.