DSMC Calculation of Vortex Shedding behind a Flat Plate with a New Intermolecular Collision Scheme

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Abstract. The generation of vortices for the flow past a flat plate is calculated by the DSMC method. The new intermolecular collision scheme and the conventional one are compared with respect to their allowable cell dimension. In the condition of *Re*=50, when using the conventional scheme, the vortex behind an inclined flat plate becomes weak with increasing the cell dimension beyond the mean free path, and finally the structure of vortex is smeared out. In the new scheme, on the other hand, the strength of the vortex does not weaken even with the cell length being ten times the mean free path. At *Re*=200, the new scheme can produce the vortex shedding behind a flat plate with the cell dimension of 20λ for the inclined plate, or 12λ in the case of a normal plate to the flow direction, although the conventional one cannot. The new intermolecular collision scheme is verified effective for unsteady flows such as vortex shedding.

INTRODUCTION

The DSMC method [1] has features different from continuum calculation methods like the finite difference method. The DSMC method has no unstable factor that a calculation diverges and has the merit that its boundary condition can be easily determined. Since the DSMC is a microscopic calculation method that deals with molecules directly, it might become possible to elucidate unstable fluid phenomena such as a turbulent flow. The most serious problem, when the DSMC method is applied to a continuum fluid, is that it is necessary to divide the flowfield into a network of cells the dimension of which is smaller than the local mean free path. At the meeting of the RGD23, one of the authors has proposed a new intermolecular collision scheme [2] in which velocities of a molecule are modified according to positions of a collision pair. Although the scheme was verified to be effective with a one-dimensional normal shock wave and with a two-dimensional vortex in a square cavity, the original version of the scheme (Usami-system-0 or U-system-0) was not perfect for an axisymmetric simulation or a 3-D simulation of a supersonic free jet and the velocity modification was obliged to be reduced to 50% of the full value because the distortion of the profile appeared with the full modification. Afterwards, the stability of the calculation was improved (even not perfect) with the addition of the limitation in the flow velocity ratio and the temperature ratio between the locations of two molecules. And also, it was found that the use of the bi-linear or the tri-linear interpolation for calculation of the temperature and the flow velocity at any location within a cell can reduce the amount of the storage required (U-system-1). In the new collision scheme the total momentum or the total energy of each collision pair is not necessarily conserved during a collision, though the overall value of all molecules can be conserved within statistical fluctuation. After various researches from such a point of view, we have found the reliable scheme (U-system-2) in which the stability improves much by an additional procedure, and the full modification of the velocity becomes possible even in an axisymmetric simulation or a 3-D simulation of a supersonic free jet where sudden changes occur of flow properties. The new collision scheme has been almost completed for steady problems, and next, it is necessary for us to investigate an effectiveness of the scheme to unsteady problems. We target a generation of vortices for flow past a flat plate. Under low Reynolds number, the steady flow past a plate at an angle of attack of 45 degrees produces one vortex behind the plate. With increasing *Re*, however, a periodic vortex separation occurs, and this is an unsteady state problem. We also apply the new collision scheme to a velocity profile in a circular tube under the condition of a turbulent flow even though it is still at a testing stage.

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NEW INTERMOLECULAR COLLISION SCHEME

The average distance between molecules of a collision pair is in proportion to the cell length when two molecules are chosen at random among molecules in the cell. If the cell length is larger than the local mean free path, the molecules that should not collide normally may come to collide, and the result of simulation may be distorted. It would be favorable that in an intermolecular collision the second molecule as a collision partner could be selected at the same location that the first molecule is selected at. In the new scheme, the velocity of a molecule being at a different location is modified as if the molecule would be located at the same position as the first selected molecule. We assume that the velocity distribution in all places is in local equilibrium, and we call two molecules P and Q that participate in the intermolecular collision. The velocity of P is one value (point A in Fig. 1) of the velocity distribution f_1 at the location of P and the velocity of Q is one value of the velocity distribution f_2 at the location of Q. To transfer the molecule P to the same position as Q, we should move the point A to the appropriate position within the velocity distribution f_2. The most natural method to move the point A into the velocity distribution f_2 is that the relative location of P within f_2 is maintained as the relative location A within f_1. This velocity modification is calculated easily. The x velocity component u_2 in f_2 (the point B in Fig.1) is calculated from the original velocity u_1 of P using Eq.(1).

$$u_2 = U_2 + (u_1 - U_1)\sqrt{T_{x2}/T_{x1}} \tag{1}$$

where U_1 and T_{x1} are the flow velocity and the temperature of f_1, and U_2 and T_{x2} are those of f_2. To use Eq.(1), it is necessary to find the temperature and the flow velocity at the location of the molecule P and also find those at the location of the molecule Q. To obtain the temperature and the flow velocity in the flowfield, we must first calculate the flow by the DSMC method using the conventional collision scheme in a coarse cell network. We call this calculation Calcu_1. The variations of the temperature and the flow velocity (along x, y, and z axes) within the cell are each approximated as a linear function. The temperature and the flow velocity at any location are calculated using the results obtained by Calcu_1. If the degree of nonequilibrium is small, the average temperature may be used such as $T_x = T_y = T_z = T$ to reduce the memory. The temperature and the flow velocity obtained by Calcu_1 must be corrected by the calculation that follows Calcu-1 and so on. In unsteady problems, especially, the time interval between Calcu_(i) and Calcu_(i+1) should be small enough that the time delay would not have a bad influence on the velocity modification. The core of an intermolecular collision calculation is the same as the conventional calculation, although using the modified velocity u_2 (v_2, w_2) of the molecule P calculated by Eq.(1). As a result, let's assume that the velocity of the molecule P changes to the point C (u_{2b}) on the velocity distribution f_2 as in Fig.1. We should bring the post-collision velocity of the molecule P to the position D (u_{1b}) on the velocity distribution f_1 because P must return back to the original location. The velocity modification is performed by Eq.(2) as in the first modification where Eq.(1) is used.

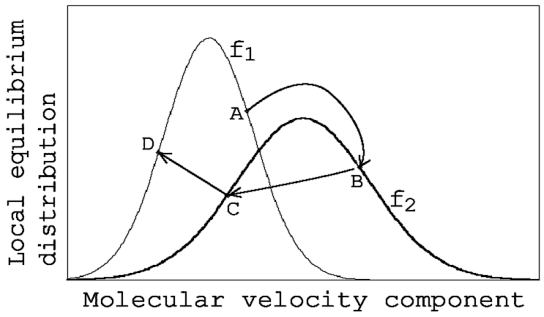


FIGURE 1. Modification of velocity in the new intermolecular collision scheme

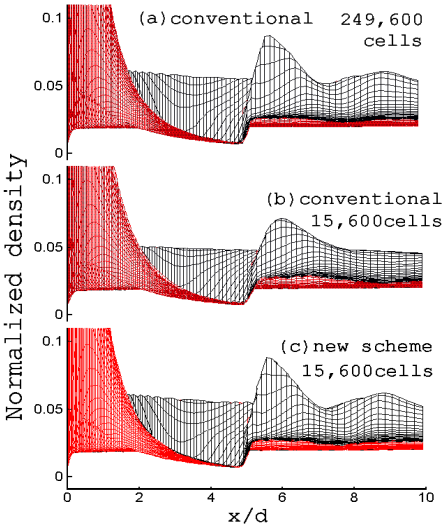


FIGURE 2. Density profiles of a supersonic free jet

$$u_{1b} = U_1 + (u_{2b} - U_2)\sqrt{T_{x1} / T_{x2}} \quad (2)$$

Note that although Eq.(1) and Eq.(2) have been derived with the assumption of equilibrium distribution functions, these equations themselves and the new collision scheme are not restricted only on equilibrium problems. In the third version of the new collision scheme (U-system-2), we impose the limitation of the ratio between flow velocities, or temperatures, at locations of two molecules as mentioned earlier. We also use a bi-linear or a tri-linear interpolation to estimate flow properties at any location within a cell. For example of the bi-linear interpolation in a two dimensional flowfield, when the temperatures of four corners (x, y), ($x+A$, y), (x, $y+B$) and ($x+A$, $y+B$) of a rectangular cell are T_1, T_2, T_3 and T_4, and the location of a molecule is ($x+a$, $y+b$), the temperature at the location of the molecule is calculated by Eq.(3).

$$T = (1-b/B)\{(1-a/A)\,T_1 + (a/A)\,T_2\} + (b/B)\{(1-a/A)\,T_3 + (a/A)\,T_4\} \quad (3)$$

In addition to that, we have found that if the change of the total energy during a collision in the two molecules exceeds a certain limit, for example, ± 10% of the pre-collision value, the probability that a distortion of results is caused by the collision pair cannot be neglected and that the new scheme should not apply to the intermolecular collision of such a pair. Although the possibility of the occurrence of the collision pair is very weak, for example, less than 0.0005, and an addition of the procedure excluding the collision pair from an application of the new scheme does not affect the efficiency of the new scheme, the stability improves much by the additional procedure and the full modification of the velocity becomes possible even in an axisymmetric simulation or a 3D simulation of a supersonic free jet. Figure 2 shows the comparison of density profiles of the axisymmetric free jet ($Kn = 3\times10^{-4}$ and pressure ratio 50) between the result by the conventional collision scheme with 249,600 cells (or 15,600 cells) and that by the new scheme with 15,600 cells, where d is a diameter of an orifice. The new scheme realizes an excellent result with very small number of cells, in other words, with very small number of molecules. Anyone who has an interest in the new collision scheme may request the Fortran source code (U-system-2) of the free jet calculation to the author through E-mail (usami@mach.mie-u.ac.jp). Figure 3 shows the density contours in two planes normal to the jet axis in the 3-D free jet analysis ($Kn = 3\times10^{-5}$ and pressure ratio 100) calculated with the new collision scheme and the conventional one. When the free jet flows through a circular orifice, since it has instability essentially, the axisymmetric structure is not maintained and a petal pattern of density contours is known to appear in a plane normal to the jet axis. The petal patterns in the jet cross sections are reproduced very clearly with the new collision scheme, but not with the conventional scheme, where 13×10^6 cells and 36×10^6 molecules are used.

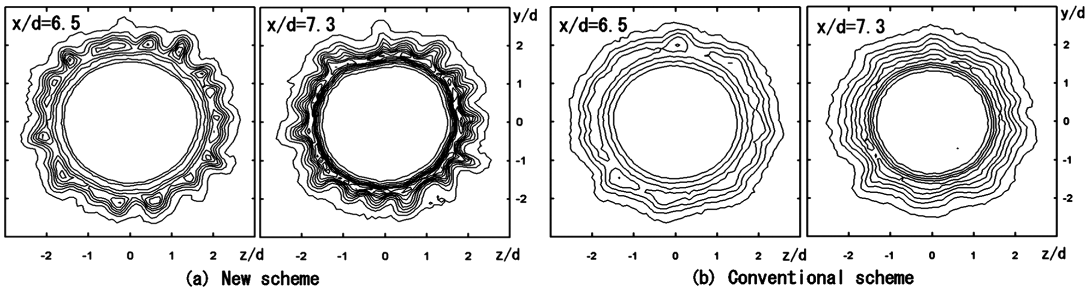


FIGURE 3. Petal patters of density contours in planes normal to the jet axis (pressure ratio 100)

RESULT AND CONSIDERATION

Steady flow past an inclined flat plate with one vortex

The vortex flow behind an inclined flat plate is a classical problem in fluid mechanics. For an uncompressible fluid, a periodic vortex separation begins to occur in the vicinity of Reynolds number Re=50. Meiburg adopted the Re number in his paper [3] where the MD method and the DSMC method were compared in respect to the manageability of vortices. In the present paper, the new collision scheme and the conventional scheme of the DSMC

method are compared with respect to their allowable cell dimension. Figure 4 shows the two-dimensional flowfield of a square ($580\lambda \times 580\lambda$) with a flat plate whose length is 60λ (2.5 mm), where λ is the undisturbed mean free path. A flow, the speed of which is 221 m/s (*Ma*=0.7), enters the flowfield at an angle of 45 degrees through a lower side boundary and a left-hand side boundary. The flowfield is divided with square cells. Three types of linear dimension of a cell are investigated: λ, 5λ and 10λ. The VHS molecule of argon is used. The pressure is 0.9 Torr, the temperature is 288 K, the *Kn* number is 0.017, and the *Re* number is 50. The total number of molecules is 840,000 in all calculations. Both schemes produce a similar steady vortex behind the inclined plate when the cell length is λ (Fig. 5(a)). In the conventional collision scheme, however, the strength of vortex becomes weak with cell length 5λ (Fig. 5(b) upper side) and the vortex disappears with cell length 10λ (Fig. 5(c) upper side). On the other hand, in the new scheme, the same strength of vortex as in the case of cell length λ is maintained even when the cell length becomes 10λ (Fig. 5 lower side).

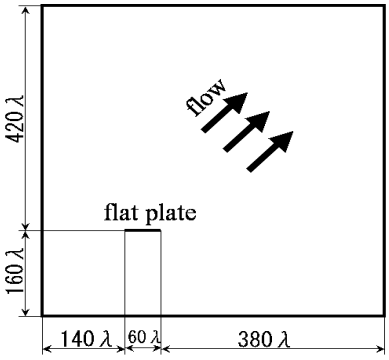
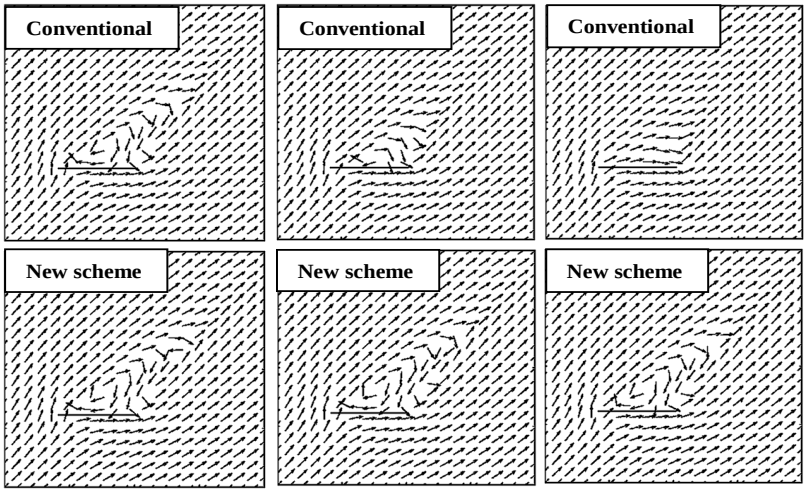
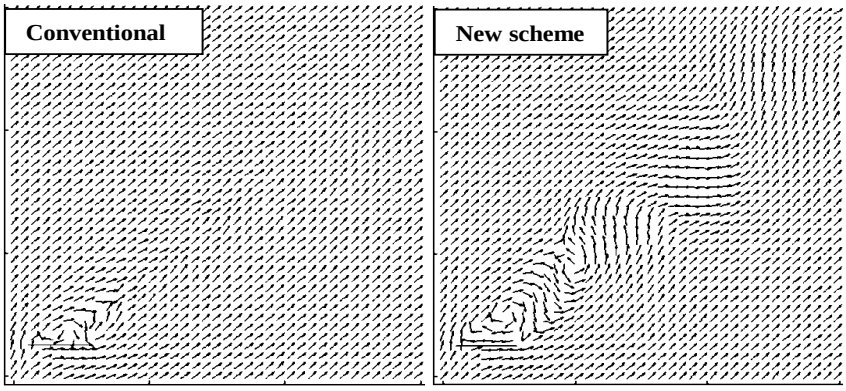


FIGURE 4. Two dimensional flowfield used to simulate vortex flows



(a) Cell length = λ **(b) Cell length = 5λ** **(c) Cell length = 10λ**

FIGURE 5. Steady vortex behind an inclined flat plate



(a) Conventional scheme **(b) New collision scheme**

FIGURE 6. Unsteady vortex flow past an inclined flat plate

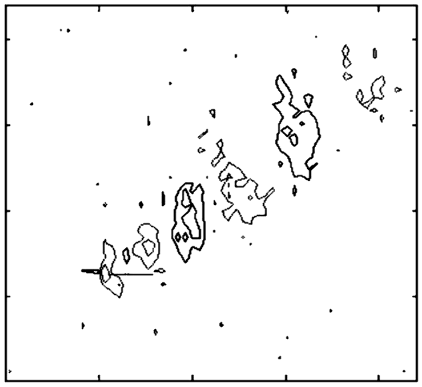


FIGURE 7. Vorticity contours behind an inclined plate by the new scheme

Unsteady flow past an inclined flat plate with vortex shedding

The steady vortex behind the inclined flat plate has been obtained at *Re*=50 as mentioned above. To produce an unsteady vortex shedding, *Re* number should be increased. For *Re*=200 (*Kn*=0.0043), the two schemes are compared

in the same flowfield as above-mentioned. The flowfield is divided with 13,456 (116×116) square cells. The linear dimension of a cell is 20λ and the length of the plate is 240λ. The pressure is 3.5 Torr. The number of molecules is 840,000. In the new scheme, the flow properties (flow velocity and temperature) are needed to modify molecular velocities. Since they must change with time in case of unsteady flows, samplings of flow properties should be done at a sufficiently short time interval compared with the time scale for changing speed of the flowfield. The present sampling interval is selected to be about one-twentieth of the characteristic time for a periodic vortex separation. Figure 6 shows the results of streamline obtained with the different collision schemes. The new collision scheme can produce a distinct vortex shedding, although the conventional scheme cannot. Figure 7 indicates vorticity contours obtained by the new collision scheme. A negative vorticity (thin lines) is produced at the left-hand side of the plate and a positive vorticity (thick lines) is produced at the right-hand side periodically, and they flow to the downstream with the passage of time. The calculation time of the new scheme in this case is about 40% greater than that compared to the conventional scheme. It has the inclination to increase with increasing density.

Vortex shedding behind a flat plate perpendicular to the flow

Periodic vortex shedding behind a flat plate perpendicular to the flow is also investigated with the two collision schemes. Figure 8 shows the rectangular flowfield that is divided with 20,000 square cells (200×100). The linear dimension of the cell is 12λ, and the length of the flat plate is 240λ. The number of molecules is 640,000. The pressure of argon gas is 4.3 Torr, the temperature is 288 K, the flow velocity is 221 m/s (*Ma*=0.7), *Re*=200, and *Kn*=0.0043. A monitoring cell in which an oscillation of flow properties is investigated is located at the center of the flowfield. Although only small flow disturbances behind the plate are found in the result of the conventional calculation (Fig. 9), regular periodic vortex shedding is clearly seen as in Fig. 10 when using the new scheme. The clockwise vortex (negative vorticity) is produced at an upper edge of the plate and the counter clockwise vortex (positive vorticity) is produced at a lower edge, alternately. They flow to the downstream keeping a certain distance between them. Figure 11 shows vorticity contours by the new scheme (thin lines are negative and thick lines are positive vorticity). An oscillation frequency of the vortex shedding can be obtained through investigating temporal variation of flow properties, especially using velocity component normal to the flow direction, in the monitoring cell. Strouhal number *St* turns out to be about 0.2, which is a reasonable value according to the published data.

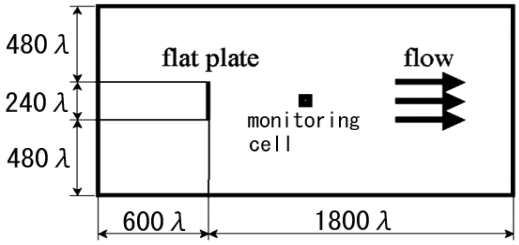


FIGURE 8. Flowfield used to simulate vortex shedding behind a normal flat plate

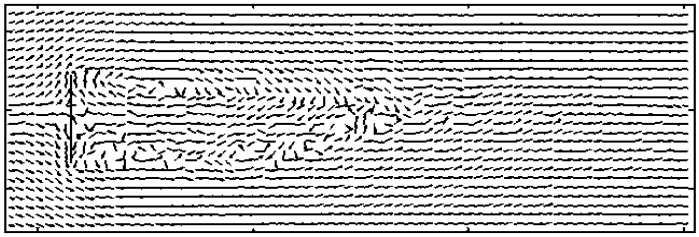


FIGURE 9. Small flow disturbances behind a normal flat plate by the conventional collision scheme

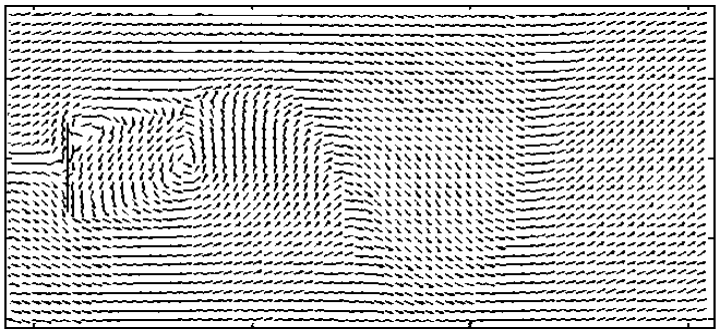


FIGURE 10. Regular vortex shedding behind a normal flat plate by the new collision scheme

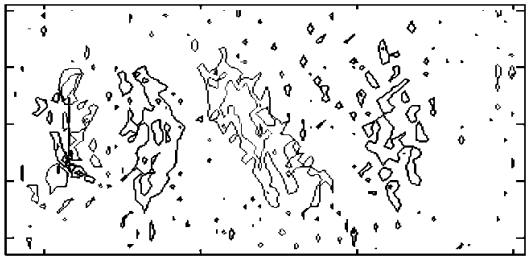


FIGURE 11. Vorticity contours behind a normal flat plate by the new collision scheme

Velocity profile in a circular tube under a turbulent flow condition

Molecular simulation on transition of flow from laminar to turbulent is one of the most interesting problems. A deformation from the velocity profile of Poiseuille flow in a cylindrical tube is investigated with the new collision scheme. This attempt is not necessarily performed by perfect algorithm based on the theoretical endorsement and it is still at a testing stage. A cross-section (*y*-*z* plane) of a circular tube is enclosed by a circumscribed quadrate that is divided by 160,000 (400×400) square cells. Only one cell is available in the *x* direction (the flow direction) and the periodic boundary condition is applied to the boundary perpendicular to the *x*-axis. The number of molecules of argon gas is about 1260,000. A diameter of the tube is 4 mm and an average flow speed is 69 m/s (0.2 times the most probable molecular speed). An initial velocity profile is parabolic. A flow speed would decrease with time because the flow suffers pipe friction. In this calculation, then, a momentum loss parallel to the pipe wall is compensated by means of giving small momentum to all molecules equally to conserve the total value. Moreover, the translational energy would be remarkably accumulated with increasing time, especially in the new collision method, and the temperature would change along the radial direction in the tube considerably. To prevent this undesirable effect, the total energy over all molecules is counted just after the intermolecular collision routine and a small energy is subtracted from, or against long odds added to, the energy of each molecule equally every time step, so that the total energy can be conserved. Enough consideration has not yet been done about an adverse effect that these artificial operations cause for this simulation. The time interval between updates of flow properties that are used for modification of molecular velocities is 3000 times the mean free time of molecular collisions. Figure 12 shows velocity profiles in the case of pressure 400 Torr ($Re \cong 10{,}000$). Though the departure of the velocity from the curve of laminar flow is apparent, since the present result is sensitive to the time interval, more careful searches about it will be needed in the future. In the conventional scheme, on the other hand, all profiles of flow velocity become parabolic irrespective of *Re*.

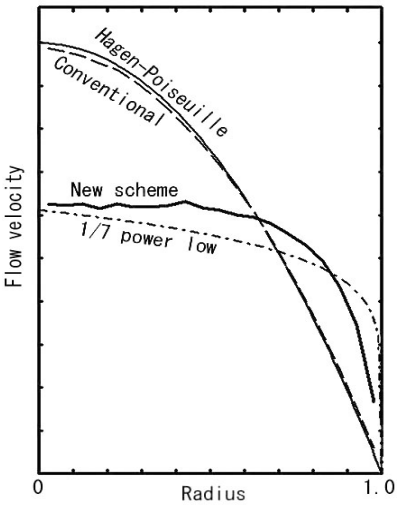


FIGURE 12. Velocity profile in a circular tube

CONCLUSION

The present paper is related to the new intermolecular collision scheme of the DSMC method and the following conclusions have been obtained.

(1) It is useful for an improvement of stability in the new collision scheme that the new scheme applies only to the collision pair whose post-collision energy is within 90% to 110% of the pre-collision value.

(2) Although the strength of steady vortex behind an inclined plate becomes weak with cell length 5λ and the vortex disappears with cell length 10λ in the conventional scheme at *Re*=50, the same strength of vortex as in the case of cell length λ is maintained in the new scheme even when the cell length becomes 10λ.

(3) In the case of cell length 20λ, the new collision scheme can produce a distinct vortex shedding behind an inclined flat plate at *Re*=200, although the conventional scheme cannot.

(4) Regular periodic vortex shedding is clearly seen behind a flat plate normal to the flow direction and Strouhal number about 0.2 is obtained at *Re*=200 when using the new scheme with cell length 12λ, although only small flow disturbances are found in the result of the conventional scheme.

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