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Simulation of Lid Cavity Flow Using Quasi-Molecular Modelling

Sitthichai KULSRI, Mullica JAROENSUTASINEE and Krisanadej JAROENSUTASINEE

CX-KURUE & Computational Science Graduate Program, School of Science, Walailak University, Nakhon Si Thammarat 80161, Thailand

ABSTRACT

We have developed a new method based on quasi-molecular modelling to simulate cavity flow. Each quasi-molecule is defined as a group of particles that interact in a fashion entirely analogous to classical Newtonian molecular interactions. When a cavity flow was simulated, the instantaneous velocity vector fields were obtained by using an inverse distance weighted interpolation method. The velocity vector fields showed the development of a primary vortex and the motion of its core from the upper right to a more central location. The results were in a good agreement with previous studies. A secondary vortex occurred at the lower right corner; however, the secondary vortex was generally difficult to locate. The velocity distributions obey the Maxwellian distribution and the configurationally internal energy fluctuated around stable average values when the systems were at equilibrium.

Keywords: Quasi-molecular modelling, particle modelling, molecular aggregate approach, lid driven cavity flow

INTRODUCTION

The simplicity of the geometry of the cavity flow makes the problem easy to code and apply boundary conditions. It follows, that the driven cavity flow is one of the most studied fluid problems in computational fluid dynamics [1]. The driven cavity flow serves as a benchmark problem and almost every new numerical method for the 2-D steady incompressible Navier-Stokes equations is tested on the driven cavity flow in terms of accuracy, and numerical efficiency [1].

Most numerical simulations of the driven cavity flow use Navier-Stokes equations. Navier-Stokes equations are fundamental equations that govern fluid flow and can solve the dynamics of water flow. However, Navier-Stokes problems are still not accessible, in either two or three dimensions when the equation of motion is in velocity components and time dependent [2-5].

Quasi-molecular modelling or particle modelling is a new numerical approach developed by Greenspan [6]. In this model, the number of molecules is scaled down from their actual values ($\sim 10^{24}$) to smaller sizes (i.e. a small set of quasi-molecular particles which is approximately $10\text{-}10^2$ particles), while the intermolecular forces are correspondingly adjusted to approximately the correct hydrodynamic situation in order to agree with classical molecular-type formulas and conserve both mass and normalised energy. Unlike the continuum and statistical mechanics approaches, this approach can be used for both steady state and non-steady state phenomena and variations in dynamical responses due to the variation of system parameters.

Quasi-molecular modelling is applied to simulate a two-dimensional cavity problem for liquids [7-9]. Primary vorteces and turbulent flows are exhibited and studied. A smoothing or filtering process, average velocities, is introduced to clarify the instantaneous velocity vector field which is dominated by Brownian type motions. Quasi-molecular modelling has the same functional form as the molecular dynamics model. The velocity distribution of particles should obey the Maxwellian distribution and the configurationally internal energy should fluctuate about stable average values [10].

In this study, we focused on a prototype fluid problem (i.e. the cavity problem). We obtained the simplicity associated with two-dimensional flow, even though our method can apply in three dimensions equally as well. This allowed us to compare our results with the numerous numerical and experimental results available in the literature. This study aimed to simulate a 2-D lid driven cavity flow in water and used cgs units throughout by using a quasi-molecular modelling, and to examine the velocity distribution of

particles which should obey a Maxwellian distribution when the system is at equilibrium.

MATERIALS AND METHODS

Quasi-molecular Modelling

Quasi-molecular modelling is used to simulate the lid driven cavity flow. The physical response of the fluid is caused by external forces (i.e. molecular interaction) [11]. In quasi-molecular modelling, the interaction forces are considered only between nearest-neighbour particles and assumed to be the same form as in molecular dynamic (MD) modelling. The interaction force is represented by Eq. (1).

$$F(R\ ) = \frac{G}{R^p} + \frac{H}{R^q} \tag{1}$$

Where G, H are parameters in the particle structure
p, q are exponential parameters in the particle structure
R is equilibrium position in the particle structure

G, H, p, q are positive constants with $q > p$ in order to obtain the repulsive effect that is necessarily stronger than the attractive one. Molecular interaction forces have two components: attraction and repulsion. The four parameters G, H, p and q are yet to be determined. If p, q and R_0 are given, then by conditions of mass and energy conservation, G and H are derived. R_0 is the equilibrium distance of the quasi-particle structure.

Just as in MD modelling, the dynamic equation of motion for each particle P_i of the system is given by Eq. (2).

$$\frac{d^2\vec{R}_i}{dt^2} = \sum_{\substack{j=1 \\ j\neq i}}^{N} \left(\frac{G}{R_{ij}^p} + \frac{H}{R_{ij}^q} \right) \frac{\vec{R}_{ij}}{\left|R_{ij}\right|},\ i \neq j \tag{2}$$

Where $\vec{R}_{ij}$ is the vector form of P_j to P_i
$\vec{R}_i$ is the position of i particle.
N is the number of particles

For the simulation of the lid driven cavity flow by quasi-molecular modelling, a two-dimensional closed square basin has a length of 6.1 cm and width of 6.1 cm (**Figure 1**). We construct a regular, triangular grid of 1098 points on the basin. The edge length of each triangular building block is 0.2 cm. We choose $p = 3$, $q = 5$, $R_0 = 0.2$ cm and the distance of local interaction $D = 3$ cm, so the motion of particle P_i is determined by Eq. (3).

$$\frac{d^2\vec{R}_i}{dt^2} = \sum_{\substack{j=1 \\ j\neq i}}^{1098}\left(-\frac{12.402}{R_{ij}} + \frac{3.100}{R_{ij}^3}\right)\frac{\vec{R}_{ij}}{|R_{ij}|} \tag{3}$$

Our model solves this equation simultaneously with a leapfrog numerical scheme.

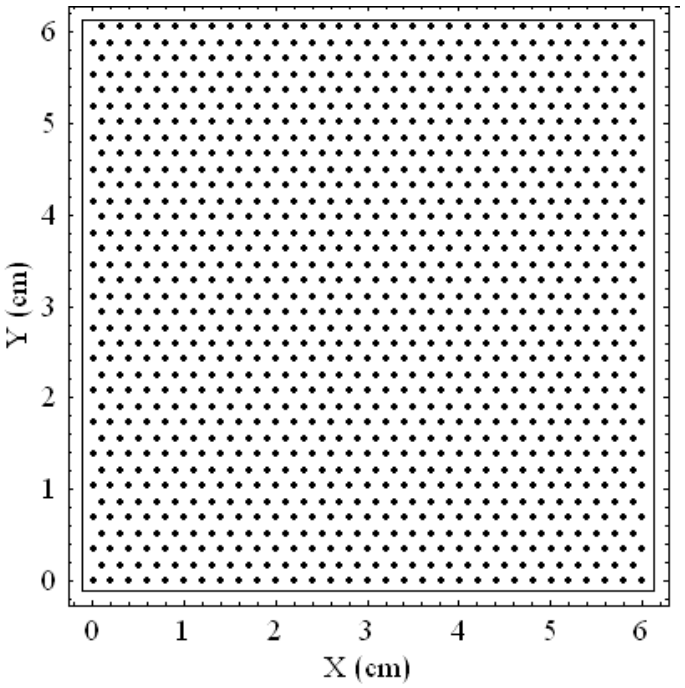


Figure 1 Configuration of 1098 water particles in the cavity.

Numerical Solution

In general, $F_i = m_i \ddot{r}_i$ (i = 1,2,3, …, N) cannot be solved analytically from the initial given data and has to be solved numerically. The choice of a numerical method is simplified by the physics of quasi-molecular modelling in small time steps. The reason is that the repulsive component H/R^q in Eq. (1) can be treated accurately only with small time steps for small R, since H/R^q is unbounded as R goes to zero. Therefore, the advantages of using a high order numerical method, which allow the choice of large time steps in obtaining a high degree of accuracy, are not applicable in quasi-molecular modelling [11]. The leapfrog formulas relating position, velocity and acceleration for particle P_i are as in Eq. (4) - (6).

$$\vec{v}_{i,1/2} = \vec{v}_{i,0} + \frac{\Delta t}{2}\vec{a}_{i,0}, \text{ (starter formula)} \tag{4}$$

$$\vec{v}_{i,k+1/2} = \vec{v}_{i,k-1/2} + (\Delta t)\vec{a}_{i,k}, \; k = 1,2,3,\ldots \tag{5}$$

$$\vec{r}_{i,k+1} = \vec{r}_{i,k-1/2} + (\Delta t)\vec{v}_{i,k+1/2}, \; k = 0,1,2,\ldots \tag{6}$$

Where $\vec{v}_{i,k}$, $\vec{a}_{i,k}$ and $\vec{r}_{i,k}$ are the velocity, acceleration and position vectors of particle i at time $t_k = k\Delta t$, Δt is the time step, $\vec{v}_{i,k+1/2}$ is the velocity of particle i at $t_k = (k+1/2)\Delta t$, and so on.

Coordinate-System Setup

A two-dimensional closed square basin has a length of 6.1 cm and width of 6.1 cm (**Figure 1**). The sides of the basin are called walls. The top wall alone is allowed to move in the X direction and has extended length so that the fluid is always enclosed by four walls. The speed V of this motion is called the wall speed (V). In the basin, a regular triangular grid with edge length 0.2 cm is constructed. The triangular grid has 31 columns and 36 rows with 1098 grid points. A regular triangular grid of 1098 points is constructed with the recursion formula.

$$\begin{array}{llll}
x_1 = 0, \; y_1 = 0, & x_{32} = 0.1, & y_{32} & = 0.1732 \\
x_{i+1} = 0.2 + x_i, & y_{i+1} = y_1, & i & = 1,2,\ldots,30 \\
x_{i+1} = 0.2 + x_i, & y_{i+1} = y_{32}, & i & = 32,33,\ldots,60 \\
x_i = x_{i-61}, & y_i = 0.3464 + y_{i-61}, & i & = 62,63,\ldots,1098
\end{array}$$

At each grid point (x_i, y_i), we set a particle P_i, that is, an aggregate of water molecules or a water particle (**Figure 1**). The water particles are distributed uniformly throughout the interior of the cavity. Then, we assign an initial random velocity over the interval [-0.5,0.5] to each particle in order to complete the initial data condition.

Simulation of Lid Driven Cavity Flow

Once all initial data are determined, the 1098 water particles are allowed to find their own equilibrium position as they interact in accordance with Eq. (3). The dynamic equations are then solved numerically by the leapfrog formula with $\Delta t = 0.00005$ and local force interactions are restricted to pairs of particles whose distance of separation are less than D = 3.0 cm. At every time step, each velocity is reduced by a factor of 0.3. In the simulation, there are three solid walls (i.e. left, right sides and the bottom) and one moving wall at the top. When a particle crosses one of the three solid walls into the exterior of the cavity, we proceed into two steps. First, the particle is reflected back symmetrically relative to the wall into the interior of the basin. Second, the velocity is multiplied by –1. However, when a particle crosses the moving wall into the exterior of the cavity, its position is reflected back symmetrically into the basin interior as before but its Y velocity component is multiplied by –1, and its X velocity component is increased by the wall speed V. In this study, we restrict the area of moving wall to 6.1×0.1 cm at the upper part of the wall. It is only when the particle moves into this area, that its X velocity component is increased by the wall speed V.

The quasi-molecular modelling has the same functional form as the molecular dynamics model. The equilibrium distribution of velocities obeys the Maxwell-Boltzmann law. The Maxwellian distribution of velocities for a two-dimensional ideal gas [9] is shown in Eq. (7).

$$N(v)dv = N\left(\frac{m}{kT}\right)ve^{-\frac{mv^2}{2kT}}dv \tag{7}$$

$N(v)dv$ is an average number of particles having velocity in the range v to $v + dv$
N is the total number of particles
m is the mass of the particles
T is the absolute temperature
k is Boltzmann's constant
v is velocity

The speed of the molecule with the average energy of kT is

$$v_{rms} = \sqrt{\bar{v}^2} = \sqrt{\frac{2kT}{m}} \tag{8}$$

Rearranging Eq. (8) we obtain

$$\frac{m}{2kT} = \frac{1}{v_{rms}^2} \tag{9}$$

Substituting Eq. (9) into Eq. (7), then

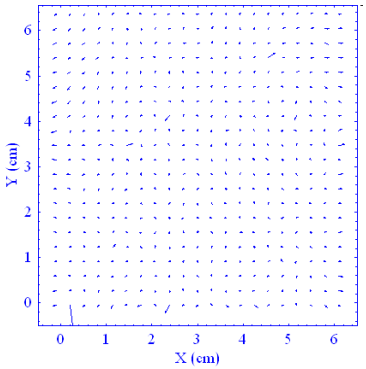
$$N(v)dv = N\left(2\frac{1}{v_{rms}^2}\right)ve^{-\frac{v^2}{v_{rms}^2}}dv \tag{10}$$

Eq. (10) is the Maxwellian distribution of velocities for two-dimensions in terms of v_{rms}.

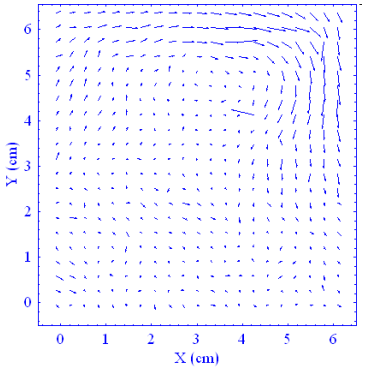
RESULTS AND DISCUSSION

Time sequences of instantaneous velocity fields from time t = 0.0000 to t = 1.2000 s are shown in **Figures 2a-h**. The velocity fields were obtained by using an inverse distance weighted interpolation method, frequently used for interpolation of scatter points [13]. **Figures 2a-h** showed the development of a primary vortex at time t = 0.0000 to t = 1.2000 s. The motion of its core moved from the upper right to a more central location (**Figures 2a-h**). The fluid motion was clockwise. The results are in good agreement with previous simulation studies [7-9]. The results from previous studies [7-9] have been verified by experimental results and numerical calculations with Navier-Stokes equations [14,15]. Their results also showed that the primary vortex developed in the upper part of the cavity and its core moved towards the centre of the cavity as the time increased. However, our primary vortex occurred in the upper right corner but in their studies it was observed in the upper left corner of the cavity. This difference could be because we used a higher upper wall velocity in our simulation than in previous studies.

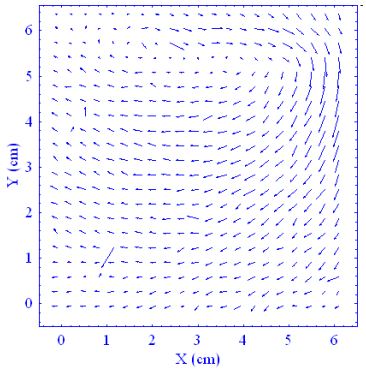
(a) *t = 0.00005 s*



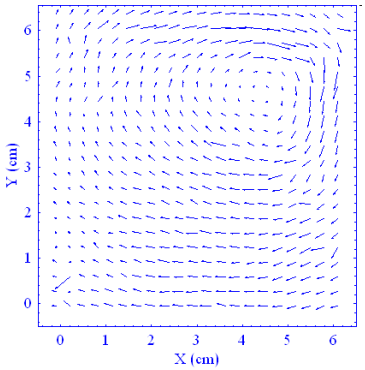
(b) *t = 0.10000 s*



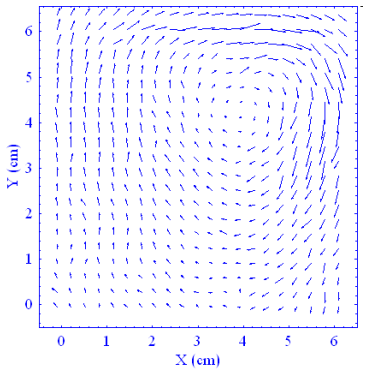
(c) *t = 0.30000 s*



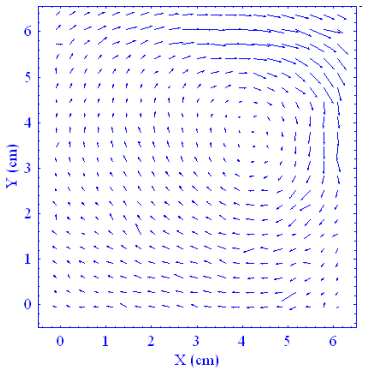
(d) *t = 0.50000 s*



(e) *t = 0.70000 s*



(f) *t = 0.90000 s*



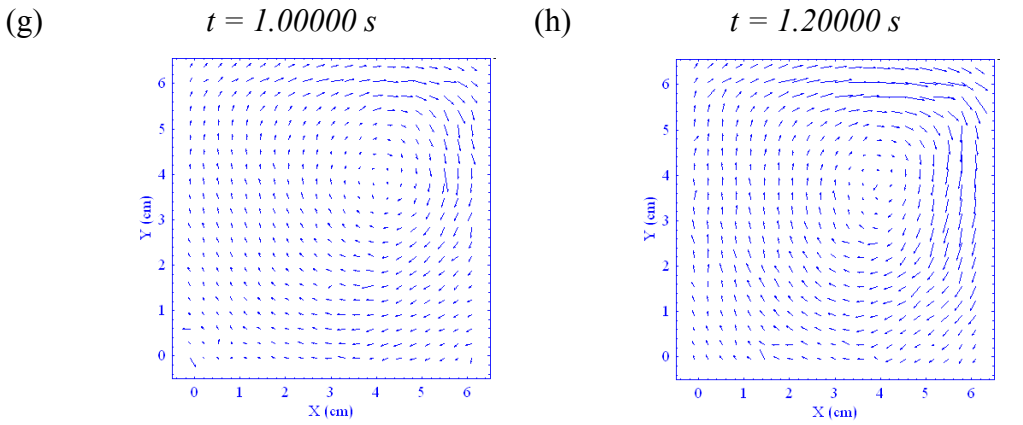


Figure 2 Time sequences of instantaneous velocity vector field. (a) *t = 0.00005* s, (b) *t = 0.10000* s, (c) *t = 0.30000* s, (d) *t = 0.50000* s, (e) *t = 0.70000* s, (f) *t = 0.90000* s, (g) *t = 1.00000* s, and (h) *t = 1.20000* s.

The secondary vortex was generally difficult to locate because the particles could be in motion and did not reveal themselves readily in a given velocity field [7-9]. With these constraints, it was very difficult to capture the secondary vortices in the simulation. However, a secondary vortex in the lower right corner at *t = 0.85000* s is shown in **Figures 3a** and **b**.

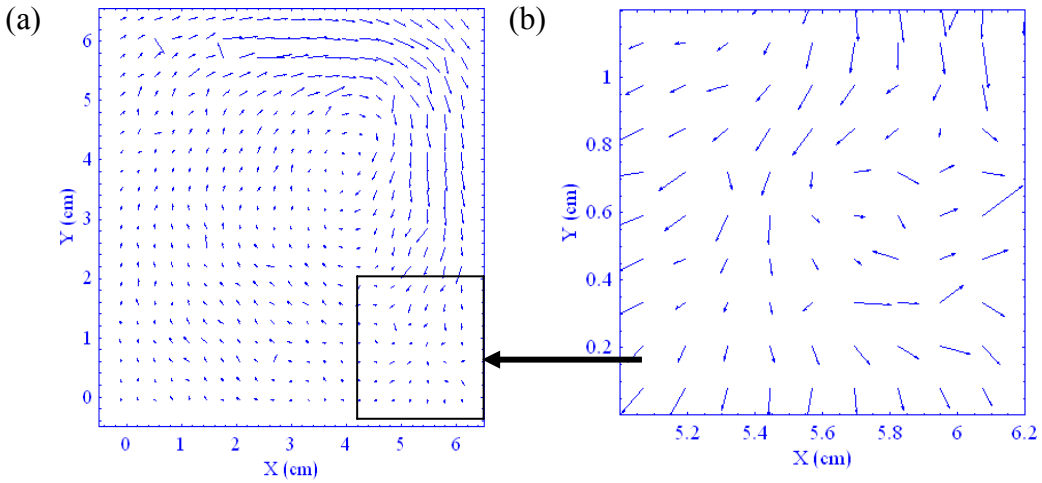
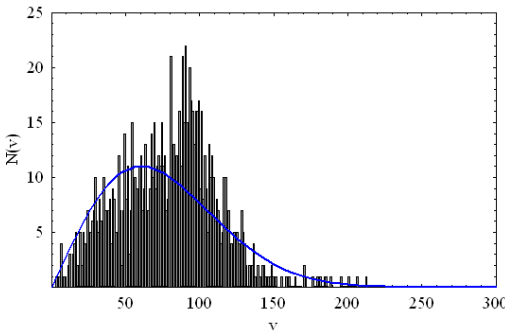


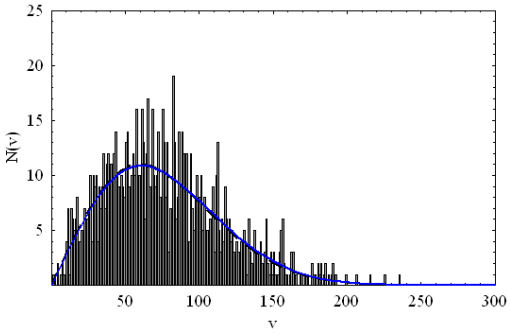
Figure 3 (a) Instantaneous velocity vector field in the cavity at time, *t = 0.85000* s. (b) Instantaneous velocity vector field in the cavity at the bottom right corner at time, *t = 0.85000* s.

After the particles were allowed to find their own equilibrium, the velocity distribution of particles obeyed the Maxwellian distribution [as in Eq. (10)]. The formation of the Maxwellian distribution from the initial velocity distribution is shown in **Figures 4a-h**. The numbers of particles at particular velocities are shown as gray bars (**Figures 4a-h**). The theoretical distribution was calculated using Eq. (10) and is shown as a dashed line (**Figures 4a-h**). The observed distribution from our simulation was calculated using a non-linear fit function in *Mathematica* and is shown as solid line (**Figures 4a-h**). The configurationally instantaneous kinetic energy fluctuated about stable average values of 6.135×10^5 ergs/particle after 0.02 s (**Figure 5**). This stable kinetic energy means that the system reached its steady state at approximately $t = 0.02$ s.

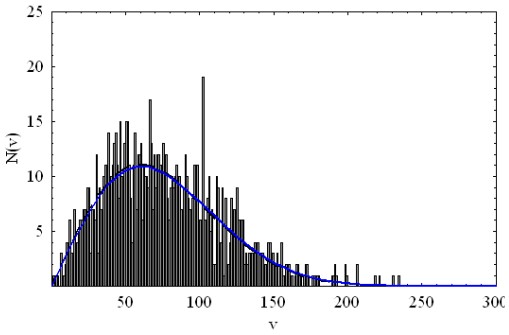
(a) *t = 0.00005 s*



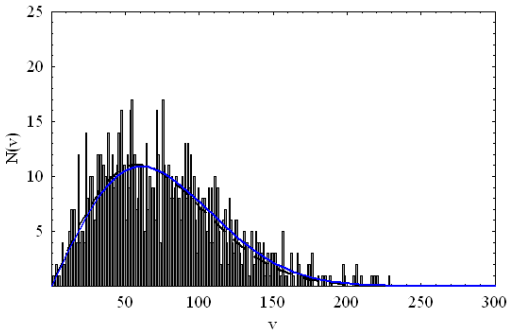
(b) *t = 0.10000 s*



(c) *t = 0.30000 s*



(d) *t = 0.50000 s*



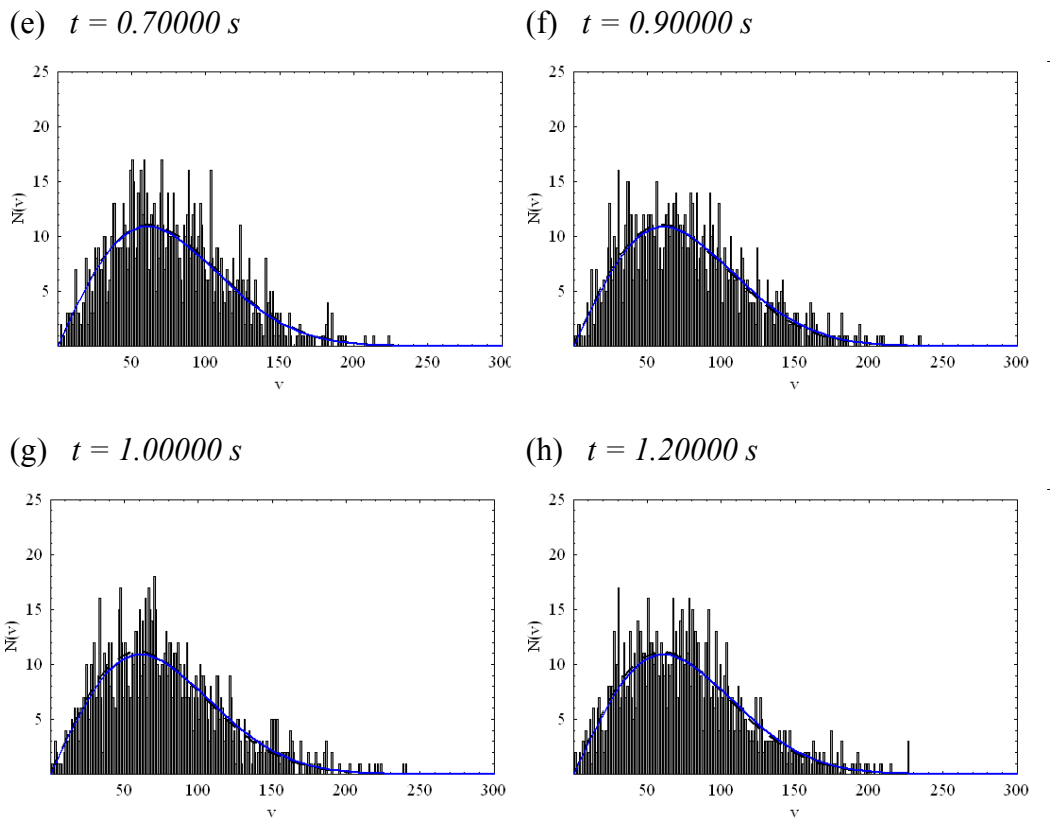


Figure 4 The time sequences of the distribution of the particle velocity. (a*) t = 0.00005* s, (b) *t = 0.10000* s, (c) *t = 0.30000* s, (d) *t = 0.50000* s, (e) *t = 0.70000* s, (f) *t = 0.90000* s, (g) *t = 1.00000* s, and (h) *t = 1.20000* s. Gray bars, solid line and dashed line represent the number of particles at given velocities, the theoretical distribution and the observed distribution, respectively.

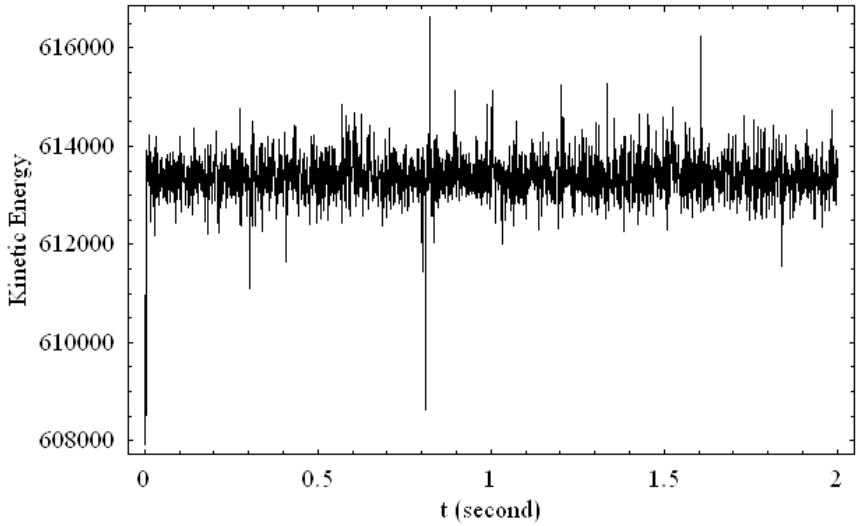


Figure 5 The instantaneous kinetic energy (ergs/particle) from a simulation of 1098 particles.

CONCLUSION

Quasi-molecular modeling is a new numerical approach that can be applied to simulate a two-dimensional cavity problem. Each quasi-molecule is scaled down from their actual value to smaller size. The intermolecular forces are correspondingly adjusted to approximately the correct hydrodynamic situation. The primary and secondary vorteces occur in the simulation. The configurationally internal energy fluctuates around stable average values when the systems are at equilibrium.

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บทคัดย่อ

สิทธิชัย กุลศรี มัลลิกา เจริญสุธาสินี และ กฤษณะเดช เจริญสุธาสินี

การจำลองการไหลของน้ำในช่องสี่เหลี่ยม โดยใช้แบบจำลองควาซิโมเลกุล (Quasi-molecular)

เราได้พัฒนาวิธีการจำลองการไหลของน้ำในช่องสี่เหลี่ยมโดยใช้แบบจำลองควาซิโมเลกุล (Quasi-molecular) แบบจำลองนี้ในแต่ละควาซิโมเลกุลประกอบด้วยกลุ่มอนุภาคที่มีอันตรกิริยากันในรูปแบบของโมเลกุลที่ทำอันตรกิริยาแบบนิวโตเนียน (Newtonian molecular interaction) ในการจำลองการไหลของน้ำในช่องสี่เหลี่ยมเราใช้วิธีการ inverse distance weighted interpolation ในการแสดงสนามเวคเตอร์ความเร็ว (velocity vector field) ในการจำลองการไหลของน้ำ สนามเวคเตอร์ความเร็วแสดงการเกิดจุดน้ำวนหลัก (primary vortex) อย่างชัดเจน ซึ่งจุดศูนย์กลางของน้ำวนอยู่ค่อนไปทางด้านขวามือด้านบนจากจุดศูนย์กลางภาพ ผลจากการจำลองนี้ใกล้เคียงกับผลการศึกษาอื่นๆที่ได้ทำการศึกษามาแล้ว สำหรับจุดน้ำวนรอง (secondary vortex) นั้นเกิดขึ้นที่มุมด้านล่าง แต่อย่างไรก็ตามจุดน้ำวนรองนั้นโดยปกติแล้วจะสังเกตได้ยาก วิธีการนี้การกระจายตัวของความเร็ว (velocity distribution) ของอนุภาคในระบบเป็นไปตามการกระจายตัวของเม็กเวลล์ (Maxwellian distribution) และเมื่อระบบเข้าสู่สภาวะสมดุล (equilibrium) พลังงานภายในระบบจะมีค่าอยู่ในช่วงของค่าเฉลี่ย

สำนักวิชาวิทยาศาสตร์ มหาวิทยาลัยวลัยลักษณ์ อำเภอท่าศาลา จังหวัดนครศรีธรรมราช 80161