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THE ROBUSTNESS ASSESSMENT FOR EVENT DRIVEN MOLECULAR DYNAMICS BY CALCULATING SPEED OF SOUND

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Abstract

Event-driven molecular dynamics (EDMD) is a special application of Molecular Dynamics (MD) derived from kinetic theory of gases. While classical solution of Navier-Stokes equations fails at high Knudsen (Kn) number flows, EDMD is valid on entire regime. Interaction potentials are considered discrete and exist only at the moment of impact. Hence, molecule trajectories are linear. Unlike the classical MD, this helps to simulate bigger systems. Molecular interactions, interaction times and partners can be predicted deterministically. Diatomic and polyatomic molecules are handled by an implemented energy relaxation scheme. Calculation of possible event times and determination of the earliest are the most time-consuming steps of the simulation. In order to improve computational speed, a cell partitioning methodology and a priority queue structure are implemented in this study. The effect of the implementations on the performance is investigated and optimum simulation parameters are determined; when using PQ, number of cells must be greater than the number of molecules for maximum computational speed. Robustness assessments for the implementations are conducted with a real-world problem. Extreme density difference in confined geometries has vast usage in engineering and is also a good example of stress test because of its complex nature. This paper addresses the calculation of sound speed in a shock tube filled with a diatomic gas by using EDMD simulations. The robustness is validated since the results agrees perfectly with the theoretical values.

Keywords: Event-Driven Molecular Dynamics Simulations, Shock tube, Sound speed, Diatomic Gases

OLAY GÜDÜMLÜ MOLEKÜLER DİNAMİĞİN SES HIZI HESABINA DAYALI SAĞLAMLIK DEĞERLENDİRMESİ

Öz

Olay güdümlü moleküler dinamik (OGMD) gazların kinetik teorisinden türetilen moleküler dinamiğin (MD) özel bir uygulamasıdır. Navier-Stokes denklemlerinin klasik çözümü yüksek Knudsen (Kn) akışlarında başarısız olurken, OGMD tüm akış rejimi için geçerlidir. Etkileşim potansiyellerinin süreksiz ve sadece temas anında mevcut olduğu kabul edilir. Bu sayede molekül yörüngeleri doğrusaldır. Bu klasik MD'nin aksine büyük sistemlerin simülasyonunu mümkün kılar. Molekül etkileşimleri, etkileşim zamanları ve çiftleri deterministik olarak öngörülebilirdir. Diatomik ve poliatomik moleküller uyarlanan bir enerji gevşeme düzeni ile modellenir. Muhtemel olay zamanlarının hesabı ve en erken olanın seçimi simülasyonun en çok zaman alan adımlarıdır. Hesaplama hızını geliştirmek amacıyla bu çalışmada bir hücre bölümleme metodolojisi ve öncelik kuyruğu yapısı simülasyona uyarlanmıştır. Uyarlamaların performans üzerine etkileri incelenmiş ve optimum süreç parametreleri belirlenmiştir; öncelik kuyruğunun kullanılması durumunda maksimum hesaplama performansı için hücre sayısının molekül sayısından fazla olması gerekmektedir. Uyarlamaların sağlamlık değerlendirmesi gerçek bir problem ile yapılmıştır. Kapalı geometrilerdeki aşırı yoğunluk farkı mühendislikte geniş bir kullanım alanı bulmakla birlikte karmaşık doğasından dolayı stres testi için uygun bir örnektir. Bu çalışma OGMD simülasyonları kullanarak diatomik bir gaz ile doldurulmuş şok tüpünde ses hızının hesaplanmasını ele almaktadır. Sonuçların teorik değerlerle mükemmel olarak uyum göstermiş olması sağlamlığı doğrulamaktadır.

Anahtar Kelimeler: Olay Güdümlü Moleküler Dinamik Simülasyonları, Şok tüpü, Ses hızı, Diatomik gazlar

Cite

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1. Introduction

Gas flow in a sub micro channels is essential in micro and nano-electromechanical systems (MEMS, NEMS). It plays an important role in the design and operation of micro-devices such as micro-pumps, micro-valves and microturbines [1]. The ratio of mean free path of gas molecules (λ) to the characteristic length of the channel (L_c) is defined as the Knudsen number ($Kn=\lambda/L_c$). Channel size is in the order of λ in micro and nano scales; flow is in between the transition regime and free molecular flow in which compressibility and rarefaction effects matters and Navier-Stokes equations are hardly valid as stated by Chapman and Cowling [2]. Similar flow regime can be observed in atmospheric re-entry problems where mean free path is too large due to low density and gravity [3]. Based on kinetic theory of the gases, such flows can be treated as an ensemble of particles which interact with each other and the boundaries. Molecular Dynamics (MD) [4–6] and Direct Simulation Monte Carlo (DSMC) [7] methods which are consistent with Boltzmann equation [8] are the ones of the most common simulation methods in the literature.

DSMC is a statistical simulation in which millions of molecules are represented with a smaller number of molecule group. Hence the method is stochastic. There are two stages in the simulation which are motion stage (deterministic) and collision stage (statistical/random). DSMC simulations are not concern of this study.

In MD simulations, all the molecular interaction times are calculated deterministically. Position and velocity of each molecule in the system are particularly known throughout the simulation. Therefore, MD yields an accurate and realistic representation of flow properties. In the classical approach of MD simulations, interaction potential between the molecules and surroundings are continuous. Hence, each potential calculation should be carried out in a feasibly small time step otherwise some interaction would be missed. The downside of this method is the computational cost of molecular interactions.

As the flow rarefies, the importance of the interaction potential decreases together with increasing average distance between molecules. For such flow, especially for monoatomic gases, molecules can be thought of as hard spheres. The potential is now discontinuous and exists only if the molecules are intact. Since each interaction is deterministically predictable and molecules continue on their trajectory between two consecutive interaction, flow can be simulated in an event-driven manner. By taking advantage of the event-driven nature together with increase in computational power and development of more effective algorithms, Event driven molecular dynamics (EDMD) simulations are now capable of simulating a larger number of molecules than before, too [9-13].

Since the monoatomic molecules have only three translational degrees of freedom, all the collisions are considered as elastic, so post-collisional velocities can be calculated simply by conservation of momentum. On the other hand, diatomic molecules undergo inelastic collisions because they have two additional rotational degrees of freedom. In Borgnakke – Larsen model, total energy at the time of the impact shared between translational and rotational modes of molecules [14].

Most of the low Knudsen number flows can be simulated with current molecule and boundary models in EDMD simulations. Efficient algorithms such as cell partitioning [11] and event scheduling [15–17] extend the size of the simulation up to several millions of molecules.

The main purposes of this study are i) investigation of the effect of the cell partitioning and event scheduling to computational performance and determination of the optimum simulation parameters, ii) robustness assessment of the EDMD simulations. Simulation of extreme density difference is a prominent way since it helps to test both physical modelling (e.g. relaxation of diatomic molecules) and implementations. Hence in this study, speed of sound in a shock tube is calculated by using EDMD simulations and validated with its theoretical value.

2. Materials and Method

2.1. Collision Modelling in EDMD simulations

For any kind of collision between two molecules A and B with masses m_A, m_B, and velocities $\boldsymbol{u_A}$, $\boldsymbol{u_B}$, relative velocity ($\boldsymbol{g}$) and centre-of-mass velocity ($\boldsymbol{G}$) are given as:

$$\boldsymbol{g} = \boldsymbol{u_A} - \boldsymbol{u_B} \tag{1}$$

$$\boldsymbol{G} = \frac{m_A \boldsymbol{u_A} + m_B \boldsymbol{u_B}}{m_A + m_B} \tag{2}$$

In a collision event, some energy is transferred between translational (e_{tra}) and rotational (e_{rot}) modes but total energy is conserved.

$$e_{tra,A} + e_{rot,A} + e_{tra,B} + e_{rot,B} = e'_{tra,A} + e'_{rot,A} + e'_{tra,B} + e'_{rot,B} \tag{3}$$

Note that rotational energy is 0 for monoatomic molecules. From conservation of mass and momentum, post-collision of molecules monoatomic molecules (no translational energy) can be calculated as

$$\boldsymbol{u'_A} = \boldsymbol{u_A} - 2\frac{\mu_{AB}}{m_A}\boldsymbol{\epsilon}\langle \boldsymbol{\epsilon}, \boldsymbol{u_A} - \boldsymbol{u_B}\rangle \tag{4}$$

$$\boldsymbol{u'_B} = \boldsymbol{u_B} - 2\frac{\mu_{AB}}{m_B}\boldsymbol{\epsilon}\langle \boldsymbol{\epsilon}, \boldsymbol{u_A} - \boldsymbol{u_B}\rangle \tag{5}$$

Here $\langle .,. \rangle$ is the inner product, μ_{AB} is reduced mass and $\boldsymbol{\epsilon}$ is unit position vector passing from the centre of the molecules at the moment of contact.

$$\mu_{AB} = \frac{m_A m_B}{m_A + m_B} \tag{6}$$

$$\boldsymbol{\epsilon} = \frac{\boldsymbol{x_A} - \boldsymbol{x_B}}{|\boldsymbol{x_A} - \boldsymbol{x_B}|} \tag{7}$$

For diatomic and polyatomic molecules, Borgnakke – Larsen energy relaxation scheme is used for inelastic collision [14]. This scheme is based on probabilistic redistribution of total collision energy between molecules according to translational and rotational degrees of freedom.

Relative translational energy is calculated as follow:

$$e_{tra} = \frac{1}{2}\mu_{AB}|g|^2 \tag{8}$$

After the collision, the total energy is conserved but distributed among modes (e'_{tra} and e'_{rot}) by an acceptance – rejection method [7]. Hence post-collision relative velocity is calculated as follow:

$$|g'| = \sqrt{2e'_{tra}/\mu_{AB}} \tag{9}$$

Finally, post-collision velocities can be expressed as

$$u'_A = G - \frac{\mu_{AB}}{m_A}|g'|\epsilon' \tag{10}$$

$$u'_B = G - \frac{\mu_{AB}}{m_B}|g'|\epsilon' \tag{11}$$

where $\boldsymbol{\epsilon}'$ is an isotropically chosen random vector from a unit sphere.

2.2. Spatial Considerations

Most of EDMD simulations as well as sound speed calculations are handled in a rectangular box along x-axis. Although many complex boundary condition models exist in the literature, only specular and periodic boundaries are required in such simulation (Figure 1); if a molecule collides with a specular wall, it bounces back with reversed normal component of its velocity vector. Tangential components remain unchanged. If a molecule reaches to a periodic boundary, it continues to its course from opposite face with its current velocity.

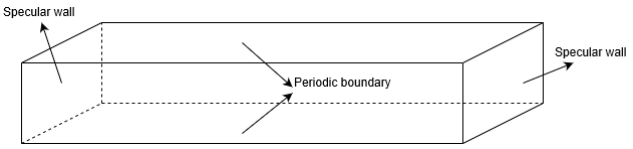

Figure 1. Spatial domain of shock tube.

Cell partitioning method [11] is applied to domain in order to increase computational speed. In the absence of cell partitioning, each molecule is a candidate collision partner of another in the domain. Hence computational complexity is O(N). With cell partitioning, domain is divided into cubical subdomains. Hence a subdomain has 27 neighbour subdomains including itself. Since a molecule can cross from one subdomain into another throughout his course, possible collision partners are only the ones exist in the neighbourhood of its own cell. This method can reduce computational complexity to O(1) with proper selection of number of molecules per cell which is one of the aims of this study.

2.3. Determination of the soonest event

A molecule can collide with both other molecules and system boundaries or cross from its own cell to one from its neighbourhood. All these particular behaviours are called events in EDMD simulations. The most time consuming process of the simulation is the determination of next event [18] and consists of two steps; i) determination of all possible event for each molecule and keeping the most recent one, ii) selection of next event among all events. Hence one must book same number of events with molecules in the simulation. In conventional EDMD simulations, generally a linear search over events is carried out. Since the complexity of linear search is O(N), it is impossible to simulate high number of molecules even with decent computers. This is one of the major fall-backs of conventional EDMD simulations. Many priority queue applications such as calendar queues [19] and ladder queues [10] for event scheduling problems exist in the literature. This study implements a priority queue proposed by Paul [15]. All events are kept in array of linear lists. According to its occurrence time, each event falls into one of the linear lists. It is not needed to keep the lists ordered except the most recent one in which a complete binary tree implementation is used to determine the most recent event. Details of the implementation can be found in the literature.

3. Results and Discussions

3.1 Performance Assessments

According to computational complexity and function calling frequencies, most time-consuming parts of EDMD simulations are the computation of collision times (*MolMolTime*), execution of collisions and determination of post-collision velocities (*MolMolCol*), cell crossings (*CellCrossing*) and determination of current event (*GetCurrentEvent*). Hence, it is essential to focus on these functions in a performance assessment of EDMD simulations. For a fair benchmarking, all the simulations are carried out in a periodically bounded cubic domains with same Kn number in this section.

Kandemir associated the determination of next event with the cell structure [11] i.e., the most recent event is determined for each cell and the global next event is the most recent one among them. After the execution of an event, it is sufficient to determine the next event of cells associated with the previous one. An average of 8 molecules per cell is the optimum for such approach [11]. Change in computational time with number of molecules is investigated for linear search in simulations (Figure 2).

When the number of molecules is low, calculation of collision times costs nearly half of the total computational time. Contribution of the current event determination is at 25% for low number of molecules but increases virtually to 100% even with a mid-sized simulation (N=592704).

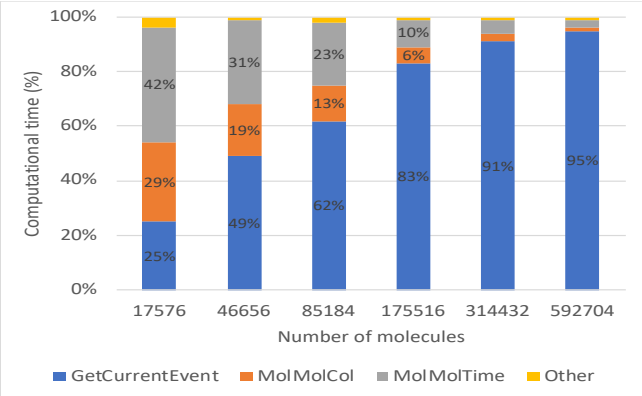

Figure 2. Computational times with linear search.

As shown in Figure 3, the result is a dramatical decrease in the performance. Event processing rate decreases up to 40 times with N=592704 compared with N=17576. Note that, actual loss of performance is much higher since the time in EDMD simulation is scaled with the number collision per particle (cpp). Elapsed time in the simulation is a function of both size of the system and event processing rate. Naturally, in small systems elapsed time for 1 cpp is shorter than in the big ones. Regarding this, slowing down ratio is in order of thousands. Practically, it is clear that it is impossible to simulate even mid-sized problems with linear search algorithm.

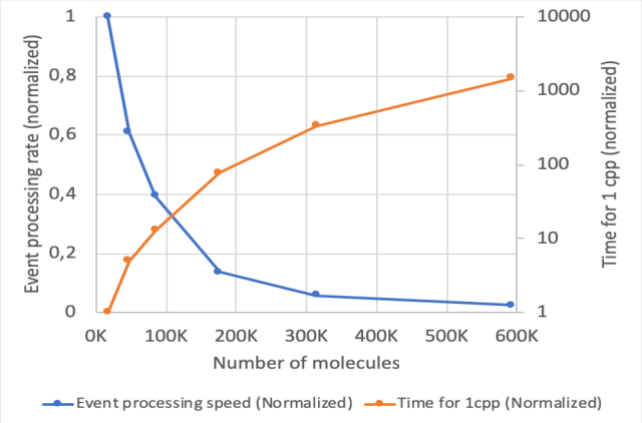

Figure 3. Computation rate with linear search.

Linear search algorithm is now replaced with a promising alternative, priority queue implementation. Contribution of the functions to the total computational time is given in Figure 4. There is an obvious progress with PQ implementation; contribution of the PQ never exceeds 5% independent from number of simulated molecules. It can be also stated that contributions of the functions are not sensitive to number of simulated molecules except the calculation of collision times which is increased from 24% (N=17576) to 30% (N=592704). Remember that number of molecules per cell is 8 in these simulations. Hence, this is an evidence of another optimum for number of molecules per cell when dealing with PQ structures.

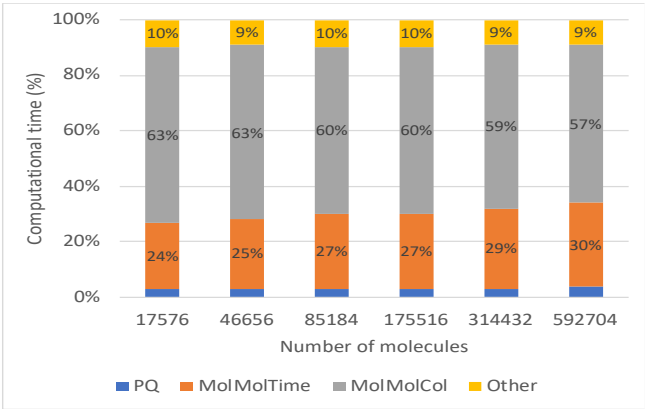

Figure 4. Computational times with PQ structure.

Effect of PQ implementation on event processing rates is given in Figure 5. Even if the number of molecules is increased 33 times, event processing rate is decreased only by half. Relation between required time for 1 cpp and number of simulated molecules is nearly linear. Hence unlike linear search algorithm, PQ implementation creates an opportunity to simulate larger systems (>1M molecules). Note that number of molecules per cell is not optimized yet and there is still room for improvement.

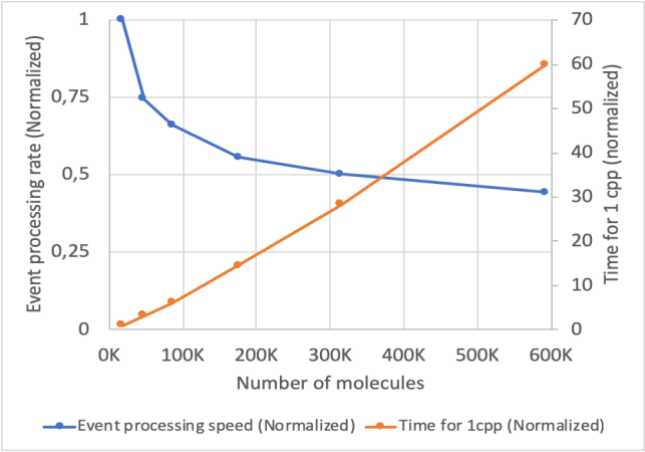

Figure 5. Event processing rate with PQ structure.

Comparison of linear search algorithm and PQ implementation as a performance ratio is given in Figure 6. For small problems (N<100k) performances of both implementations are comparable, ratio is just 6 in favor of PQ. When dealing with high number of molecules this ratio goes up to 70.

Another concern in performance assessments of EDMD simulations is the effect of cell partitioning and determination of optimum number of molecules per cell. In a non-partitioned simulation, a molecule can go a collision with any other molecule in the system so potential collision time for each pair should be calculated. Hence, contribution of the function to the total computational time is at max. Event processing rate is too low even in small systems (N<10000) (Figure 7).

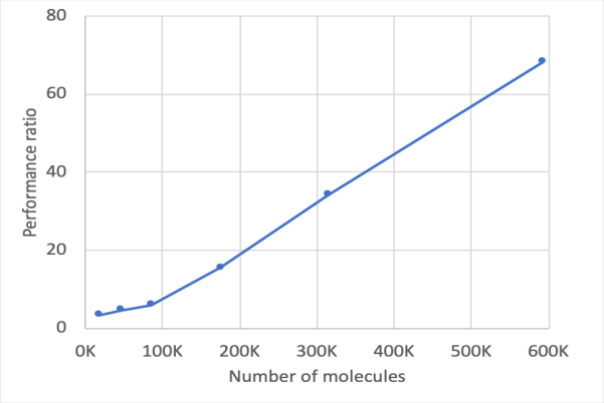

Figure 6. Performance comparison of linear search and PQ structure implementations.

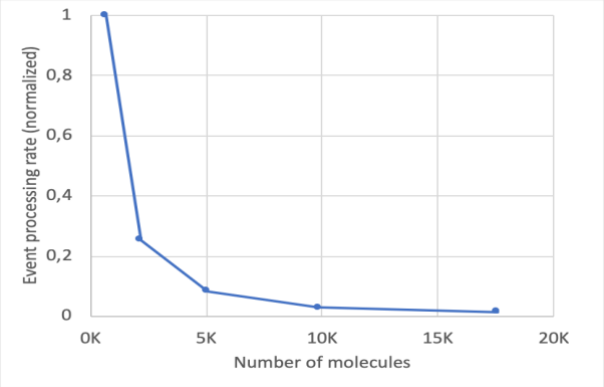

Figure 7. Event processing rate without cell partitioning.

Number of molecules per cell which is the ratio of total number of molecules to number of cells is the key parameter of the performance of cell partitioning. If the earliest event for each cell is kept and a linear search is carried over the cells, it is expected that the number of cells is lesser than the number of molecules (i.e. number of molecules per cell is greater than unity) for a smaller list of candidates. Kandemir stated that for such configuration optimum number of molecules per cell is 8 [11]. On the other hand, since there is more potential collision partner contribution of regarding function to the total computational time is high.

In the presence of PQ implementation, the complexity of current event determination is O(1). Therefore, length of the candidate list is insignificant and contribution of regarding function is already minimized. A new optimum value of number of molecules per cell should be determined accordingly. Simulation results of a mid-sized problem ($N \approx 175000$) are given in Figure 8. When number of molecules per cell is less than unity, there are fewer possible collision partner and the contribution of regarding function is lesser. On the other hand, number of cell crossing events naturally is increasing at high number of cells and its contribution is becoming dominant. With same reasons, contribution of PQ implementation is insignificant at lower number of cells but increases up to 12% when number of molecules per cell is 0.086.

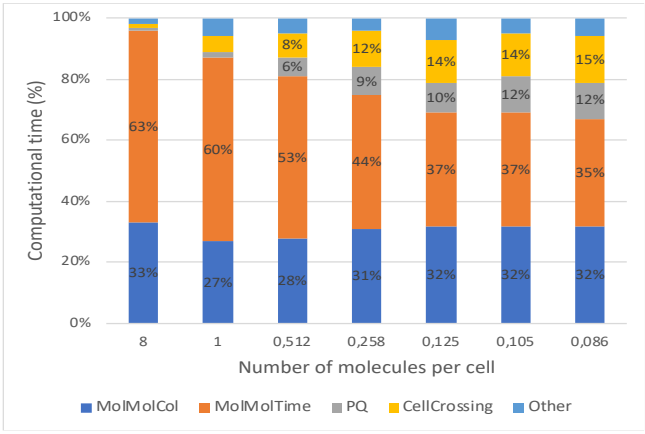

Figure 8. Computational times with cell partitioning

The effect of cell partitioning on the computational speed is given in Figure 9. Although simulation is getting faster together with decreasing number of molecules per cell, there is a natural limit; diameter of a molecule cannot be greater than the cell size. Unrelated to the problem physics but number of cells is limited in hardware aspect too. Since each cell is an instance of Cell class, it occupies some memory in computer memory. Overflowing may occur in big simulations (N>5000000). Even though event processing rate is high, contribution of cell crossing events begin to dominate total number of events as the number of cells increases. Hence it can be seen that collision processing rate maximizes around 0.25 molecules per cell.

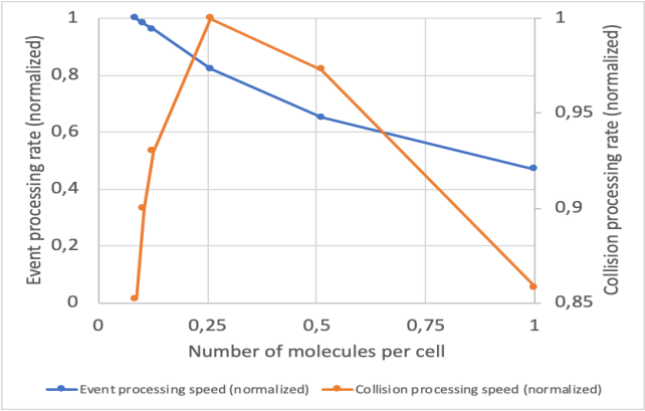

Figure 9. Effect of number of molecules per cell.

3.2 Shock Tube Simulations

After the implementation of cell partitioning and priority queue based event searching algorithms into EDMD simulations, it is essential to validate the physical modelling and assess the robustness of the simulation.

Extreme density differences are common for stress testing of molecular simulations. The result is shock wave formation and propagation which is an important phenomenon in rarefied gas dynamics and deserves an extensive examination. However, a simple shock tube simulation is a perfect test case within the scope of this study.

The idea is to deduce the sound of speed from the result of simulations. As in the study of Kandemir for

monoatomic gases [11], if the calculated value converges to the theoretical one, consistency of the implementations is ensured. This paper extends that for diatomic gases.

The theoretical value of the speed of sound (c_{the}) is:

$$c_{the} = \sqrt{\frac{\gamma k_b T}{m}} \tag{12}$$

Here, γ is the ratio of heat capacities at constant pressure and volume and 7/5 for diatomic gases. Mass of N_2 (m) is 4.616×10^{-26} kg. Boltzmann constant (k_b) is equal to $1.38064852 \times 10^{-23} m^2 kg s^{-2} K^{-1}$. Temperature (T) is selected 300 K for this study. Then the theoretical value of sound speed, c_{the} can be calculated as follows:

$$c_{the} = \sqrt{\frac{\frac{7}{5} \times 1.38064852 \times 10^{-23} \times 300}{4.616 \times 10^{-26}}} \tag{13}$$

$$c_{the} = 354.43\ m/s \tag{14}$$

A simulation of 60000 N_2 molecules confined in a 1 μm channel at 300 K temperature was conducted in order to simulate a shock tube. The spacing ratio which is the ratio of molecular spacing (s) to the molecular diameter (d) is 3.5. Simulation details are given in Table 1.

Table 1. Shock wave simulation.

Molecule	N_2
# of molecules	60000
Temperature	300K
Channel width	1 μm
Aspect ratio (width/height)	10
Spacing Ratio (s/d)	3.5

Initially, the channel is divided with virtual membrane and molecules are placed in the left half while the other half is totally empty. In order to maintain thermal relaxation, molecules are allowed to make specular collision until 10 collisions per molecule (cpp). After that, the virtual membrane is removed, and molecules are allowed to pass to the initially empty half. Hence, the development of a shock structure is expected.

The simulation is continued up to 300 collisions per molecule. While the shock wave propagates back and forth, the densities at both ends of the tube converge into an average value. Of course, such late-time oscillation should agree with the speed of sound. In a given time interval (1 cpp), the density of the gas along the tube is calculated and fitted to a $\rho(x) = ax + b$ line using least squares method (Figure 10). Variation of parameters a and b is shown in Fig. 2. Note that, a and b are time dependent and b is equal to the density at location $x = 0$.

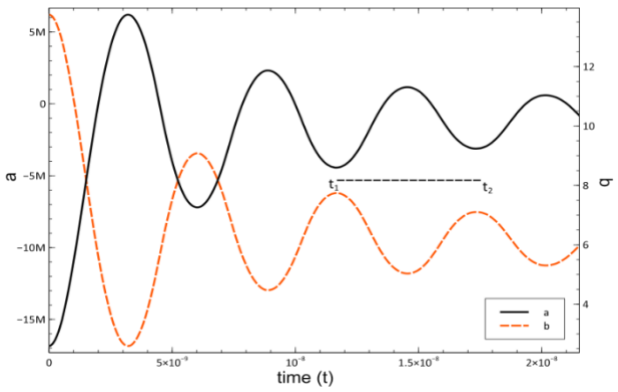

Figure 10. Time evolution of shock wave.

Sound wave goes back and forth from one end to the other and travels a total distance of two times of tube length ($2L_x$) in a peak to peak time interval shown in the Figure 10. Hence the speed of sound (c_{sim}) can be calculated as

$$c_{sim} = \frac{2L_x}{t_2 - t_1} \tag{15}$$

$$c_{sim} = \frac{2 \times 1\mu m}{(1.45605 - 0.89179) \times 10^{-8} s} \tag{16}$$

$$c_{sim} = 354.45\ m/s \tag{17}$$

Since the theoretical and calculated value of sound speed are virtually identical, it can be concluded that the robustness of the simulation and its implementations are assured.

4. Conclusion

The effects of cell partitioning methodology and priority queue implementation for event driven molecular dynamics simulation are investigated. Simulation results prior to implementations show that performing linear search for earliest event and checking possible collision pairs over entire computational domain pairs are bottlenecking computational speed and make impossible to simulate even the mid-sized systems.

Domain partitioning helps to reduce the number of possible collision partners of molecules. Besides that, it is also useful to increase the speed of linear search to a certain degree, if the number of cells is greater than number of molecules.

Implementation of priority queue structure makes a significant breakthrough in determination of earliest event. Contribution of the implementation to the total computational time is minor. It is also insensitive to the number of simulated molecules; therefore, simulations of bigger systems are possible now. Simulation results point out that the number of molecules per cell should be less than unity in the presence of PQ structure in order to minimize checking possible collision partners. Optimum value of number of molecules per cell is around 0.25

Robustness of implementations has been assessed with the calculation of sound speed in a shock tube. Simulation result is virtually identical with the theoretical one. Hence, one can say that event driven molecular dynamics

simulations and the implemented methodologies and structures work effectively and depicts realistic behaviour of the extreme conditions such as shock formation. Although periodic and specular boundary conditions are adequate for such kind of simulations, for many other engineering cases, proper wall models should be implemented into the simulation.

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