Corpuscular method for airbag deployment simulations

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ABSTRACT

A corpuscular method for simulating the flow of a gas mixture and its interaction with flexible structures has been developed and implemented in LS-DYNA. The gas mixture is represented by a set of particles obeying the laws of kinetic molecular theory. The method has been developed for airbag deployment simulations where complex gas-fabric interaction creates numerical difficulties for continuum based methods. This article briefly describes the basic theory upon which the method has been built.

INTRODUCTION

A continuum based approach to the modelling of airbag gases and their interaction with the airbag fabric has proven subjected to several difficulties. There are geometrical complexities that are hard to handle, both in the gas-fabric contact and in the treatment of gas flowing through narrow gaps.

As an attempt to circumvent those difficulties a corpuscular method for gas dynamics has been developed and implemented in LS-DYNA. The corpuscular approach is based on the kinetic gas theory. That is, a set of assumptions regarding the gas behavior on molecular level that, on a macroscopic statistical level, leads to the ideal gas law.

The corpuscular approach is Lagrangian, which simplifies the gas-fabric contact treatment. In addition, the lack of field equations greatly simplifies the development of a numerically robust implementation of the governing equations.

KINETIC GAS THEORY

The kinetic gas theory is the study of gas molecules and their interaction (on a microscopic level) which leads to the ideal gas law (macroscopic relationships). The theory is based on the following assumptions:

- The average distance between the molecules is large compared to their size.

- There is a thermodynamical equilibrium, i.e. the molecules are in random motion.
- The molecules obey Newton's law of motion. Relativistic and quantum mechanical effects are negligible.
- The only molecule-molecule and molecule-structure interactions are perfectly elastic collisions.

The kinetic theory of gases dates back to 1738 when Daniel Bernoulli [1], [2] proposed a theory that the air pressure against a piston is built up by discrete molecular collisions. Having the kinetic gas theory as a starting point, in 1860 James Clerk Maxwell [3] elegantly derived an expression for the molecular velocity distribution at thermal equilibrium. He managed to bring more understanding to details about the molecular interaction in an ideal gas. One can, from his statistical descriptions, derive quantities such as mean free path and frequency of collision.

PRESSURE

Assume one single molecule with mass m_i and velocity $\mathbf{v}_i = [v_{x,i}, v_{y,i}, v_{z,i}]^{\mathrm{T}}$ inside a rectangular box with side lengths L_x, L_y and L_z, see Figure 1.

The frequency at which this particle will impact the wall in positive x-direction becomes

$$f = \frac{|v_{x,i}|}{2L_x} \tag{1}$$

Since the impacts are assumed elastic the transferred impulse at each impact is

$$j_{x,i} = 2m_i|v_{x,i}| \tag{2}$$

Over time, the total impulse transferred to the wall becomes

$$J_{x,i} = f j_{x,i} t = \frac{m_i v_{x,i}^2 t}{L_x} \tag{3}$$

Hence, the average pressure against the wall is

$$p_{x,i} = \frac{J_{x,i}}{At} = \frac{m_i v_{x,i}^2}{V} \tag{4}$$

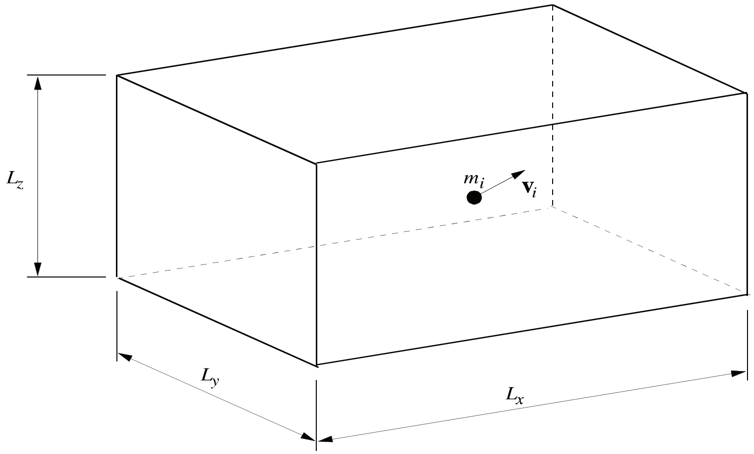

Figure 1: Molecule moving around in a box

where $A = L_y L_z$ and $V = L_x L_y L_z$ is the volume of the box. Having N particles the pressure becomes

$$p_x = \frac{1}{V}\sum_{i=1}^{N} m_i v_{x,i}^2 \tag{5}$$

At thermal equilibrium the kinetic energy will be evenly distributed between the different Cartesian directions.

$$\bar{v_x^2} = \bar{v_y^2} = \bar{v_z^2} = \frac{1}{3}\bar{v^2} \tag{6}$$

where $\bar{v^2}$ is the mean square of the molecular velocities and $\bar{v_x^2}, \bar{v_y^2}$ and $\bar{v_z^2}$ are the mean-square velocities in the different Cartesian directions. Equations (5) and (6) gives

$$p = p_x = \frac{1}{V}\sum_{i=1}^{N} m_i v_{x,i}^2 = \frac{1}{3V} m\bar{v^2} = \frac{2W_k}{3V} = \frac{2}{3} w_k \tag{7}$$

where m is the total mass of all molecules, W_k is the total translational kinetic energy of the particles and w_k is the specific translational kinetic energy. That is, at thermodynamic equilibrium there is a direct relationship between the pressure and the specific translational kinetic energy of the gas. Macroscopically this translational kinetic energy is part of the internal energy of the gas. For a mono-atomic gas w_k is actually equivalent to the total specific internal energy e, as virtually no energy is stored as molecular spin or vibrations. This gives us the following relation for a mono-atomic gas

$$p = \frac{2W_k}{3V} = \frac{2}{3}w_k = \frac{2}{3}e \tag{8}$$

Note that the pressure in ideal gas with constant heat capacities can be expressed as

$$p = (\frac{C_p}{C_v} - 1)e \tag{9}$$

Consequently, following Equations (8) and (9) $\gamma = C_p/C_v = 5/3$ for a mono-atomic gas.

ADIABATIC EXPANSION

Assume the same particle, this time inside a slowly expanding box according to Figure 2. The particle will lose some energy each time it impacts the moving wall.

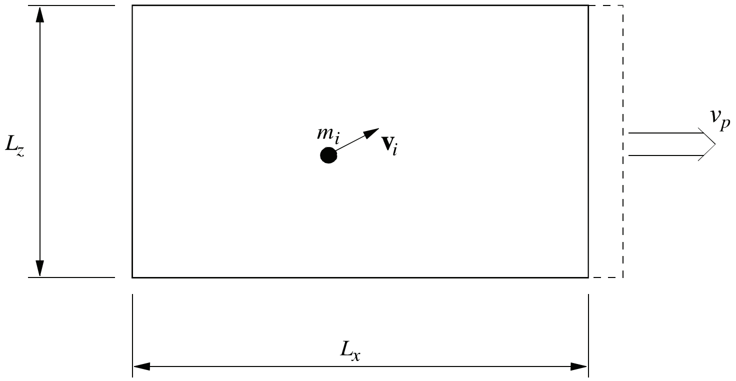

Figure 2: Molecule moving around in a box

$$\Delta E_i = \frac{1}{2} m_i (v_{x,i} - 2v_p)^2 - \frac{1}{2} m_i v_{x,i}^2 \approx |v_p << v_{x,i}| \approx -2 m_i v_{x,i} v_p \tag{10}$$

Combining this with the impact frequency in Equation (1) gives a rate of dropping energy

$$\dot{E}_i = f \Delta E_i = -\frac{m_i v_{x,i}^2 v_p}{L_x} = -m_i v_{x,i}^2 \frac{\dot{V}}{V} \tag{11}$$

Having many particles inside the box the total rate of dropping energy, due to impacts against the moving wall, becomes

$$\dot{E} = \sum_{i=1}^{N} E_i = -\sum_{i=1}^{N} m_i v_{x,i}^2 \frac{\dot{V}}{V} = |\text{Equation (6)}| = \frac{2W_k}{3} \cdot \frac{\dot{V}}{V} \tag{12}$$

W_k is a fraction ξ of the total energy E. Note that $\xi = 1$ for a mono-atomic gas. Hence, Equation (12) gives us

$$\dot{E} = -\frac{2\xi E}{3} \cdot \frac{\dot{V}}{V} \Rightarrow \left| \begin{array}{c} \text{assume temperature} \\ \text{independent } \xi \end{array} \right| \Rightarrow E(V_t) = E(V_0) \left(\frac{V_0}{V_t} \right)^{\frac{2\xi}{3}} \tag{13}$$

Here V_0 and V_t are the volumes at time 0 and t, respectively. The exponent $2\xi/3$ is actually equivalent to $\gamma - 1$. Hence, the fraction of internal energy stored as translational kinetic energy can be expressed as

$$\gamma - 1 = \frac{2\xi}{3} \Rightarrow \xi = \frac{3}{2} (\gamma - 1) \tag{14}$$

It is to be noted that temperature dependent heat capacities complicates the expressions in Equations (13) and (14).

TEMPERATURE

One definition of temperature T is that it is proportional to the average translational kinetic energy of the molecules in the gas.

$$T = \frac{M\bar{v^2}}{3R} \tag{15}$$

where M is the molar weight and $R = 8.3145 J/molK$ is the universal gas constant. Note that $\bar{v^2}$ represents the mean square velocity of particles having the same molecular weight. Large molecules move slower than small molecules at the same temperature. The relationship in Equation (15) is important when converting given temperature data to molecular (particle) velocities at the inflator nozzle in an airbag simulation.

CORPUSCULAR METHOD IN LS-DYNA

The corpuscular method in LS-DYNA is based on the kinetic gas theory. However, it is not realistic to model every single molecule inside an airbag (roughly $10^{23} - 10^{24}$). The need for computational efficiency in the numerical implementation has lead to the following assumptions and deviations from the kinetic gas theory:

- The particles are given a spherical shape (speeds up contact treatment).
- Each particle represents many molecules.
- For each individual particle there is a balance between kinetic energy and spin+vibration energy. This balance is determined directly from the heat capacities, $C_v(T)$ and $C_p(T)$.
- To obtain a smoother pressure distribution the impulse transfer from particle-fabric collisions is slightly smeared out in time.

NUMERICAL EXAMPLE

As a simple numerical example $1g$ of air at temperature $300K$ inside a rigid cubic box with side length $0.1m$ was simulated using $N = 1000$, 10000 and 100000 particles. The molar mass and the heat capacity at constant pressure were set to $M = 28g/mole$ and $C_p = 1000J/kgK$, respectively. The time step size in the simulations was $0.8\mu s$.

According to Equation (15) the theoretical root-mean-square velocity of the particles at thermal equilibrium is

$$\sqrt{\bar{v^2}} = \sqrt{\frac{3RT}{M}} = 517m/s \tag{16}$$

At this velocity it will take a particle roughly $0.2ms$ to travel from one end of the box to the other. However, unless defining very few particles the average mean free path is considerably smaller than the box size $0.1m$. Hence, few particles are like to travel across the box along one straight line. Actually, Table 1 shows the number of particle-particle collisions and particle-wall impacts over a period of $1ms$. For $N = 1000$ the average rate of collision for each particle is roughly $10ms^{-1}$. For $N = 10000$ and $N = 100000$, the frequencies are $37ms^{-1}$ and $138ms^{-1}$, respectively.

Figure 3 shows the pressure response against the inner walls (total area of $600cm^2$). The particle velocity distribution at thermal equilibrium is displayed in Figure 4.

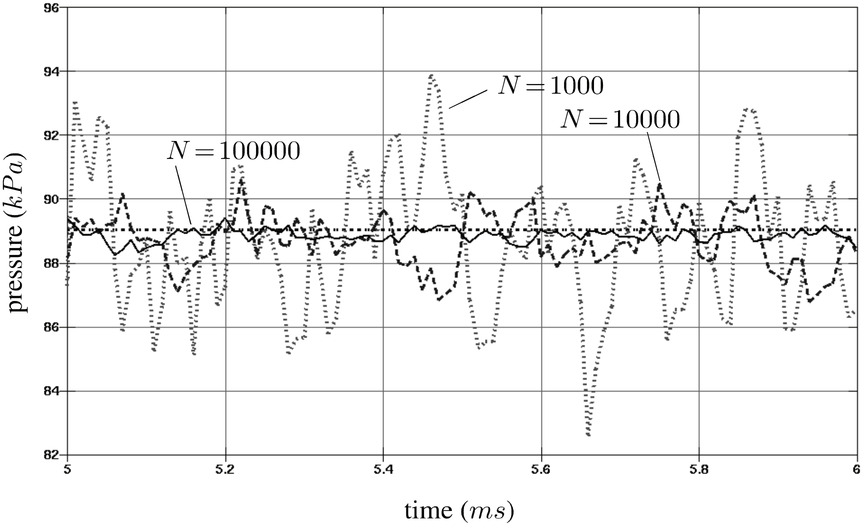

Figure 3: Pressure time history in a $1ms$ window using different number of particles. The analytical value is $89kPa$.

N	p-p	p-w
1000	4877	7102
10000	184483	70769
100000	6940980	714688

Table 1: Number of particle-particle (p-p) and particle-wall (p-w) collisions at thermal equilibrium during a period of $1ms$.

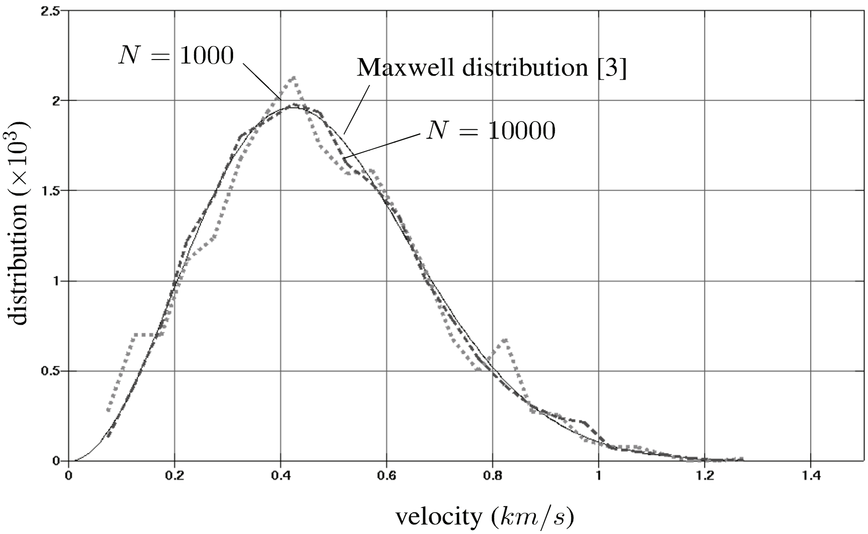

Figure 4: Snapshot of particle velocity distribution after reaching thermal equilibrium (time $5ms$)

REMARK

The corpuscular approach to gas modelling that has been implemented in LS-DYNA has its main advantage in situations of geometrically complex gas-structure interaction. In most other situations of macroscopical gas flow it is not a competitive alternative to continuum based methods.

The simple numerical example shows that some pressure oscillations are unavoidable, even at a state of thermal equilibrium.

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