Introduction to the DS-BGK Method for Gas Flow in Vacuum Systems

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1. Division of gas flow regime

\[ Kn = \frac{\lambda}{L}, \quad \lambda \approx \frac{1}{\sqrt{2\pi n}} \frac{16\mu}{5\sqrt{mkT}/\pi} \approx 65\text{nm at STP} \]

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BGK equation is a good approximation to the Boltzmann equation
2. DSMC method and Boltzmann equation

Boltzmann equation:

\[
\frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial x_j} = \int_{-\infty}^{\infty} \int_{0}^{4\pi} (f' f_1' - f f_1) c_r \sigma d\Omega d\vec{c}_1
\]

\[
\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t}|_{\text{move}} + \frac{\partial f}{\partial t}|_{\text{coll}}
\]

\[
\frac{\partial f}{\partial t}|_{\text{move}} = -c_j \frac{\partial f}{\partial x_j}
\]

\[
\frac{\partial f}{\partial t}|_{\text{coll}} = \int_{-\infty}^{\infty} \int_{0}^{4\pi} (f' f_1' - f f_1) c_r \sigma d\Omega d\vec{c}_1
\]
Another way to understand DSMC

In DSMC method:

\[ f_m = \sum_{l=1}^{Num_m} \frac{N_l}{V_m} \delta(\vec{c} - \vec{c}_l) \]

\[ \Delta f_{\text{move}} = \Delta t \left( \frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial c_j} \right) \]

\[ \Delta t: \quad \Delta f_{\text{coll}} = \frac{\Delta t n^2}{2} \iiint \left[ (\delta_2' + \delta_1' - \delta_2 - \delta_1) c_r \sigma_T \right] \frac{\sigma}{\sigma_T} \frac{f_1}{n} \frac{f_2}{n} d\Omega d\vec{c}_1 d\vec{c}_2 \]

\[ = \sum_{j=1}^{M} \left[ \frac{N_l}{V_m} (\delta_2' + \delta_1' - \delta_2 - \delta_1) \frac{c_r \sigma_T}{[c_r \sigma_T]_{\text{max}}} \right]_j, \quad M = \frac{\Delta t n^2}{2} \frac{V_m [c_r \sigma_T]_{\text{max}}}{N_l} \]

\[ N_l = N_{\text{cons}}, \text{ adjust } \vec{c}_l \text{ to record } \Delta f_{\text{coll}} \]

Disadvantages of the DSMC method

DSMC method is successful in high velocity case, but it is very time-consuming in low velocity case as in MEMS due to:

1. CPU time for generating a lot of random numbers;
2. CPU time for getting huge samples to reduce statistical noise.
3. DS-BGK method and BGK equation

Motivations of the DS-BGK method [1]:

1. Avoid using random number in intermolecular collision process
2. Retain the basic advantages of DSMC method

3. DS-BGK method and BGK equation

BGK equation

Boltzmann equation:
\[
\frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial x_j} = \int_{-\infty}^{\infty} \int_{0}^{4\pi} f' f_{1r}' c_r \sigma d\Omega d\vec{c}_1 - f \int_{-\infty}^{\infty} \int_{0}^{4\pi} f_{1r} c_r \sigma d\Omega d\vec{c}_1
\]

BGK equation [1]:
\[
\frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial x_j} = \nu (f_{eq} - f)
\]

\[
f_{eq} = n_{eq} \left( \frac{m}{2\pi k T_{eq}} \right)^{3/2} \exp\left[\frac{-m(\vec{c} - \vec{u}_{eq})^2}{2kT_{eq}}\right]
\]

\[
n_{eq} = \int_{-\infty}^{\infty} f d\vec{c}, \quad \vec{u}_{eq} = \frac{1}{n_{eq}} \int_{-\infty}^{\infty} \vec{c} f d\vec{c}, \quad T_{eq} = \frac{2}{3k} \frac{1}{n_{eq}} \int_{-\infty}^{\infty} \frac{m(\vec{c} - \vec{u}_{eq})^2}{2} f d\vec{c}
\]

\[
\mu_{BGK} = \frac{nkT}{\nu}, \quad \kappa_{BGK} = \frac{5k}{2m} \frac{nkT}{\nu}
\]

Inspirations from the Lagrangian form

\[
\frac{df}{dt} = \frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial x_j} = \nu (f_{eq} - f)
\]

1. Use \( F_l \) to record the evolution of \( df / dt \)

2. Change \( N_l \) to record \( \Delta f_{coll} \)

3. \( N_l \) can be updated according to \( N_l / F_l = cons \)
Extension of acceptance-rejection scheme

Original scheme:

assume $[\bar{x}_l, \bar{c}_l]_{all} \ l$ is a representative sample of $f_{\text{max}}$, remove $[\bar{x}_l, \bar{c}_l]$ if $f_l / f_{\text{max}} < R_f$ or retain it otherwise, the retained $[\bar{x}_l, \bar{c}_l]_{\text{retained}} \ l$ is a representative sample of $f$.

Extended scheme:

if $[\bar{x}_l, \bar{c}_l, N_l]_{all} \ l$ is a representative sample of $f_1$,

$[\bar{x}_l, \bar{c}_l, N_l (f_2 / f_1)_l]_{all} \ l$ is a representative sample of $f_2$. 
### Difference between DSMC and DS-BGK

**DSMC method**

1. constant \(N_l\)
2. carry \(\vec{x}_l, \vec{c}_l\)
3. change \(\vec{c}_l\) to record \(\Delta f_{\text{coll}}\)
4. use \(\vec{x}_l, \vec{c}_l, N_l\) to update \(n_{eq}, u_{eq}, T_{eq}\)
5. need random number for \(\Delta f_{\text{coll}}\)

**DS-BGK method**

variable \(N_l\)

carry \(\vec{x}_l, \vec{c}_l, N_l, F_l\)

change \(N_l\) to record \(\Delta f_{\text{coll}}\)

use \(\vec{x}_l, \vec{c}_l, \Delta N_l\)

needn’t for \(\Delta f_{\text{coll}}\)

High efficiency of DS-BGK method is attributed to features 4 and 5.
Algorithm of DS-BGK method

before encountering the boundary

\[
\begin{align*}
\vec{x}_l(t) & \quad \Rightarrow \quad \vec{x}_l(t + \Delta t) = \vec{x}_l(t) + \Delta t \vec{c}_l(t) \\
\vec{c}_l(t) \quad & \Rightarrow \quad \vec{c}_l(t + \Delta t) = \vec{c}_l(t) \\
F_l(t) \quad & \Rightarrow \quad F_l(t + \Delta t) = f_{eq}(t) + [F_l(t) - f_{eq}(t)] \exp(-\nu \Delta t) \\
N_l(t) \quad & \Rightarrow \quad N_l(t + \Delta t) = N_l(t) F_l(t + \Delta t) / F_l(t) \\
f_{eq}(t) \quad & \Rightarrow \quad f_{eq}(t + \Delta t) \text{ by an auto-regulation scheme}
\end{align*}
\]

\([\vec{x}_l, \vec{c}_l, N_l]_{all \ l} \text{ is always a representative sample of } f(t)\)
Boundary conditions

\[ \vec{c}_l = \vec{c}_r \text{ as in DSMC, meanwhile } F_l = f_B(t, x_r, c_r) \]

\[
f_{B,CL} = a \frac{1}{\sqrt{\pi \alpha_\tau}} \exp\left[-\frac{(c_{r,2}^* - \sqrt{1 - \alpha_\tau c_{i,2}^*})^2}{\alpha_\tau}\right]. \frac{1}{\sqrt{\pi \alpha_\tau}} \exp\left[-\frac{(c_{r,3}^* - \sqrt{1 - \alpha_\tau c_{i,3}^*})^2}{\alpha_\tau}\right].
\]

\[
\frac{1}{\pi \alpha_n} \exp\left[-\frac{c_{r,1}^* + (1 - \alpha_n)c_{i,1}^*}{\alpha_n}\right] \int_0^{2\pi} \exp\left[\frac{2(1 - \alpha_n c_{r,1}^* c_{i,1}^*)}{\alpha_n} \cos \theta \right] d\theta
\]

\[ \vec{c}^* = \vec{c} / \sqrt{2kT_{wall} / m}, \quad a \text{ is determined by } Num_r = Num_i \]

\[
Num_i = n_{eq} \sqrt{\frac{kT_{eq}}{2\pi m}} \left\{ \exp\left[ -\left( \frac{-u_{eq,1}}{\sqrt{2kT_{eq} / m}} \right)^2 \right] + \sqrt{\pi} \frac{-u_{eq,1}}{\sqrt{2kT_{eq} / m}} \left[ 1 + \text{erf} \left( \frac{-u_{eq,1}}{\sqrt{2kT_{eq} / m}} \right) \right] \right\}
\]

\[
Num_r = \int_{c_{r,1} > 0} f_{B,CL} c_{r,1} d\vec{c}_r = a(2kT_{wall} / m)^2
\]
Auto-regulation scheme

\[ n_{eq,m}^{new} = \frac{n_{eq,m}^{old} V_m - \sum_{\text{cell } m} \Delta_m N_l}{V_m} \]

\[ \rightarrow_{new} u_{eq,m} = \frac{n_{eq,m}^{new} V_m}{n_{eq,m}^{new} V_m} \]

\[ T_{eq,m}^{new} = \frac{n_{eq,m}^{new} V_m 3k / 2}{n_{eq,m}^{new} V_m} \]

Note: \( m \) is the subscript for the index of cells or as the variable for the molecular mass.
Discussion about the auto-regulation scheme

It makes \( \sum_{\text{cell } m} \Delta_m N_l, \sum_{\text{cell } m} \Delta_m N_l \mathbf{c}_l, \sum_{\text{cell } m} \Delta_m N_l \frac{m c^2_l}{2} \rightarrow 0 \) and then

\[
\int_{-\infty}^{\infty} \nu (f_{eq}^{tr} - f) \psi_k (\mathbf{c}) d\mathbf{c} = 0, \psi_1 = 1, (\psi_2, \psi_3, \psi_4) = \mathbf{c}, \psi_5 = c^2,
\]

which means \( n_{eq}, \mathbf{u}_{eq}, T_{eq} \) converge to their solutions of the BGK equation.

It uses \( \Delta_m N_l \) instead of the transient \( N_l \) and so can reduce the statistical noise due to discontinuous events of molecules moving into or out from the concerned cell.
4. Verification and efficiency of DS-BGK

Case 1. Couette gas flow

Argon gas, $T_0 = 273.15K$

$n_0 = 2.6847 \times 10^{25} \text{ m}^{-3}$

$\lambda_0 \approx 63 \text{ nm}, \Delta t = 4.3 \times 10^{-11} \text{ s}$

$Kn = \frac{\lambda_0}{D}$, adjust $D$

$T_{wall} = T_0$
Verification and efficiency of DS-BGK

Velocity and shear stress

200 cells for $Kn = 0.01$; 20 cells for $Kn = 0.1$ and 1
Verification and efficiency of DS-BGK

Case 2. lid-driven gas flow

Argon gas, $T_0 = 273.15K$, 
$n_0 = 2.6847 \times 10^{25} \text{ m}^{-3}$
$
\lambda_0 = 63 \text{nm}, \Delta t = 4.3 \times 10^{-11} \text{s}$
$W = L, \ Kn = \lambda_0 / L$

$T_{\text{wall}} = T_0$

adjust $L$
Verification and efficiency of DS-BGK

DSMC: solid line, DS-BGK: dashed line; $Kn = 0.063$, $U = 20 m/s$, $20 \times 20$ cells
4. Numerical results

Verification and efficiency of DS-BGK

DSMC: solid line, DS-BGK: dashed line; \( Kn = 0.63 \) \( U = 20 \) m/s \( 20 \times 20 \) cells
Verification and efficiency of DS-BGK

DSMC: solid line, DS-BGK: dashed line;  $Kn = 6.3$, $U = 20m/s$, $20 \times 20$ cells
4. Numerical results

Verification and efficiency of DS-BGK

DS-BGK: 7 minutes CPU time for $U=20\text{m/s}$ and $0.1\text{m/s}$, $Kn=0.063$. DSMC: 30h for $U=20\text{m/s}$ and may need $30(20/0.1)^2$ h for $U=0.1\text{m/s}$. 
4. Numerical results

Verification and efficiency of DS-BGK

Case 3. channel gas flow

Argon gas, $T_0 = 273.15K$

$n_0 = 2.6847 \times 10^{25} m^{-3}$

$\lambda_0 \approx 63 nm$, $\Delta t = 4.3 \times 10^{-11} s$

$Kn = \frac{\lambda_0}{D}$, adjust $D$

$n_{in} = n_0$, $n_{out} = 0.6n_0$

$T_{wall} = T_0$
4. Numerical results

**Verification and efficiency of DS-BGK**

**Evolution of real molecule number**

DSMC:
\[ \sum_{m=1}^{\text{all}} \sum_{\text{cell } m} N_{\text{cons}} \div \sum_{m=1}^{\text{all}} n_0 V_m \]

DS-BGK (nonuniform, left):
\[ \sum_{m=1}^{\text{all}} \sum_{\text{cell } m} N_l \div \sum_{m=1}^{\text{all}} n_0 V_m \]

DS-BGK (uniform, right):
\[ \sum_{m=1}^{\text{all}} n_{eq,m} V_m \div \sum_{m=1}^{\text{all}} n_0 V_m \]

DS-BGK: nonuniform (left) and uniform (right, 8000 simulated molecules per cell), \( Kn=0.63 \)

nonuniform: \( N_{l,\text{init}}^{\text{inlet}} = N_{l,\text{init}}^{\text{outlet}} = \text{cons} \); uniform: \( N_{l,\text{init}}^{\text{inlet}} / n_{\text{inlet}} = N_{l,\text{init}}^{\text{outlet}} / n_{\text{outlet}} \)
4. Numerical results

**Verification and efficiency of DS-BGK**

**Evolution of real molecule number**

DSMC: \[ \sum_{m=1}^{\text{all}} \sum_{\text{cell } m} N_{\text{cons}} / \sum_{m=1}^{\text{all}} n_0 V_m \]

DS-BGK: \[ \sum_{m=1}^{\text{all}} \sum_{\text{cell } m} N_l / \sum_{m=1}^{\text{all}} n_0 V_m \]

DS-BGK: \[ \sum_{m=1}^{\text{all}} n_{eq,m} V_m / \sum_{m=1}^{\text{all}} n_0 V_m \]

DS-BGK: uniform (left, 800 per cell) and (right, 80 per cell), \( Kn=0.63 \)
Verification and efficiency of DS-BGK

DSMC: solid line, DS-BGK: dashed line, $Kn=0.63$, $\alpha_r = \alpha_n = 1$, $50 \times 20$ cells
Verification and efficiency of DS-BGK

DSMC: solid line, DS-BGK: dashed line, $Kn=0.63$, $\alpha_t = \alpha_n = 0.98$, $50 \times 20$ cells
Verification and efficiency of DS-BGK

DSMC: solid line, DS-BGK: dashed line, $Kn=1.3$, $\alpha_T = \alpha_n = 1$, 50x20 cells
4. Numerical results

Verification and efficiency of DS-BGK

- DSMC: solid line
- DS-BGK: dashed line

Kn = 1.3, \( \alpha_r = \alpha_n = 0.98 \), 50x20 cells
5. Conclusions

1. DS-BGK method agrees well with DSMC method in high $Kn$ case;
2. DS-BGK method is very efficient for low velocity case;
3. Application of CLL boundary condition in DS-BGK is convenient.