# DENSITY BASED SENSITIVITY ANALYSIS OF RAREFIED GAS FLOWS USING THE DISCRETE VELOCITY METHOD

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Material interpolation scheme and sensitivity analysis are studied in this research, with the aim to achieve topology optimization of rarefied gas flow structures. Choosing the discrete velocity method as the numerical approach for the Boltzmann equation, material interpolation scheme is developed by correcting the convection flux of the discretized convection equations and re-scaling the relaxation term of the Shakhov gas kinetic model. With the proposed interpolation scheme, material distribution can be effectively modelled using a pseudo design density. A discrete adjoint system is proposed for sensitivity analysis. The governing equation, the Boltzmann equation, in the optimization problem is replaced by the steady state condition of the numerical scheme. The discretized version of the governing equation results in a simple and straightforward way to formulate an adjoint system using the Lagrangian multiplier method. The numerical solution of the original system is transposed. Numerical examples confirm the validity of the proposed methods, which can serve as the basis for structural optimization algorithms in rarefied flow systems.

*Key Words*: Boltzmann Equation, Adjoint System, Sensitivity Analysis, Rarefied Gas, Topology Optimization

#### 1. Introduction

According to the kinetic theory, gas is made up by an enormous number of molecules travelling randomly in space. Each molecule carries momentum and energy, and their random collisions result in dissipation of momentum and energy in the form of shear force and heat flux. Under usual conditions, the shear number of gas molecules guarantees that the collision frequency is extremely high, so that the mean free path (the average distance travelled by molecules between collisions) is very small, and hence negligible compared to the characteristic length of the flow field. In other words, in the macroscopic scale (one that is comparable with the characteristic length of the flow field), gas can be treated as a continuum, where only a few macroscopic quantities (such as density, temperature, and velocity) are required to fully describe it. The dissipation of momentum and energy via the numerous inter-molecular collisions can be categorically described by constitutive laws such as Newton's law of viscosity and Fourier's law of heat conduction.

However, under what is called the rarefied condition, behavior of gas can be drastically different. By definition, rarefication refers to the condition where the mean free path  $\lambda$  becomes non-negligible compared to the characteristic length  $L_c$  of the flow field. Or, introducing the non-dimensionalized Knudsen number  $\text{Kn} = \lambda/L_c$ , when Kn gets larger than  $10^{-4(1)}$ . Under rarefied conditions, the lack of inter-molecular collisions means the velocity distribution of gas molecules deviates from the conventionally assumed equilibrium conditions. As a result, the empirical constitutive conditions will break down, and the flow field will be more susceptible to the conditions of the solid boundaries that enclose it. When Kn is sufficiently large, peculiar phenomenon such as

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thermal transpiration will  $occur^{(2)}$ .

The condition of rarefication usually requires extremely low pressure (for large  $\lambda$ ) or very small spatial scales (for small  $L_c$ ). Although rarely encountered in daily life, rarefied gas are commonly found in several cutting-edge engineering fields, such as vacuum technology, space technology, and micro-electro-mechanical systems (MEMS). Accurate modelling and numerical simulation of rarefied gas flows are, therefore, of fundamental significance to the design and developments of various products. Examples include micro actuators, gas sensors, and space  $nozzles^{(4)}$ . However, the optimal design of these fascinating devices have long been an open question. This is primarily due to the mathematical and computational barriers associated with the governing equation, the Boltzmann equation. As is mentioned, rarefied gas behaves unconventionally, and thus the Navier-Stokes-Fourier (NSF) equations cannot be used as the governing equation. The Boltzmann equation employs a distribution function f to describe the distribution of gas molecules in terms of both position and velocity, and the equation is closed by considering the changes to f due to streaming, reflection, and collision of all the molecules. Over the years, several numerical methods have been developed for the Boltzmann equation, such as the direct simulation Monte-Carlo  $(DSMC)^{(5, 6)}$  the discrete velocity method  $(DVM)^{(7, 8)}$ , and the lattice Boltzmann method (LBM)<sup>(9, 10)</sup>. However, solving the Boltzmann equation numerically does not fully address the question of optimal design. Theoretically, empirical methods like trial-and-error can be applied, where one chooses from a finite number of candidates according to numerical results<sup>(12)</sup>. But clearly, empirical methods lacks rigorousness, as it cannot rule out the possibilities of better designs that are not tested yet. Apart from that, empirical methods require considerable computational resources, which makes applications to large-scale systems expensive  $^{(11)}$ . As a result, at the time being, most flow devices in rarefied flow fields have rather simple shapes, consisting mostly of straight lines and  $\operatorname{arcs}^{(13)}$ .

In order to develop optimal design approaches for rarefied gas flows, researchers have turned to topology optimization. The advantages of topology optimization is quite obvious: it preserves the high degree-of-freedoms of the original design problem, and ensures global optimality of the obtained result. However, the complexity of Boltzmann equation poses a challenge to conduct material sensitivity analysis. From the available literature, Sato et al. used a direct extension of the Boltzmann equation to describe material distribution, and design sensitivity is obtained using the adjoint variable method and the Lagrangian multiplier method<sup>(14)</sup>. However, the complexity of the Boltzmann equation, or the substituted Bhatnagar-Gross-Krook (BGK) equation, results in cumbersome derivation and numerical treatment of the adjoint system. As is reported, optimization of a 2D system using 100  $\times$  100 square meshes takes around 40 hours.

Guan et al. used direct simulation Monte-Carlo (DSMC) to calculate the rarefied flow field, and proposed a material interpolation scheme based on the DSMC algorithm using a pseudo design density<sup>(16)</sup>. For sensitivity analysis, a discretize-then-optimize (DTO) approach due to Caflisch<sup>(15)</sup> is used. This approach focuses on the dependencies of the numerical variables in the simulation, and bypasses the tedious treatment of the continuous adjoint system as is used by Sato et al. Nevertheless, the DTO approach in sensitivity analysis could require storage of all the intermediate variables during the simulation, which incurs extreme memory usage in practical terms.

In this paper, we would like to present an efficient sensitivity analysis approach for rarefied gas flows, which addresses the drawbacks of the above-mentioned methods. The structure of this paper is as follows. In Section 2, a brief review of the discrete velocity method (DVM) is provided, which is a deterministic method for the Boltzmann equation. In Section 3, a new material interpolation scheme is proposed. The proposed interpolation scheme is based on the DVM algorithm, and directly captures the presence of solid by modifying the convection fluxes. In Section 4, design sensitivity is derived based on a discrete adjoint system. It will be shown that the proposed approach reduces memory cost compared to the DTO approach, and its computational cost is comparable to the forward DVM process. Finally, in Section 5, several numerical examples are provided to validate the proposed interpolation scheme and sensitivity.

# Review of the Boltzmann equation and DVM The Boltzmann equation

Neglecting external force, the single-species rarefied gas flow is governed by the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_x f = W[f]. \tag{1}$$

In Eqn. (1), f is the distribution function of the gas molecules.  $f(\boldsymbol{x}, \boldsymbol{v}, t)$  represents the probability density of finding a molecule around position  $\boldsymbol{x}$  with velocity  $\boldsymbol{v}$  at time t. On the right hand side (RHS), W[f] is the collision integral, which describes the rate of change in f due to the collisions between molecules. The general expression for W[f] is

$$W[f] = \int_{\mathbf{R}^3} \int_{\mathcal{S}^2} q(\mathbf{v} - \mathbf{v}_1, \sigma) (f^* f_1^* - f f_1) d\sigma d\mathbf{v}_1, \quad (2)$$

where  $S^2$  is the unit sphere,  $q(\boldsymbol{v} - \boldsymbol{v}_1, \sigma)$  is the collision section that characterizes the likelihood of collision between

molecules with velocity  $\boldsymbol{v}$  and  $\boldsymbol{v}_1$  at reflection angle indicated by  $\sigma$ , and  $f_1, f^*, f_1^*$  are short-hand notations for the fat pre-collision and post-collision velocity points. The details of Eqn. (2) can be found in reference<sup>(17)</sup>.

### 2.2. DVM

In order to solve Eqn. (1), DVM first introduces a simplification of the collision integral W. The Shakhov gas-kinetic equation is often used, where

$$W[f] = \frac{1}{\tau}(f^{\rm sh} - f).$$
 (3)

In Eqn. (3),  $\tau = \mu/p$  is a characteristic relaxation time, where  $\mu$  is viscosity and p is pressure.  $f^{\rm sh}$  is a target relaxation state given through the Maxwellian distribution  $f^{\rm ma}$ by

$$f^{\rm sh} = f^{\rm ma} \left[ 1 + (1 - \Pr) \frac{\boldsymbol{Q} \cdot \boldsymbol{c}}{5p \mathsf{R}_0 T} \left( \frac{\boldsymbol{c}^2}{\mathsf{R}_0 T} - 5 \right) \right], \qquad (4)$$

where c = v - V is the peculiar velocity, Pr is the Prandtl number,  $R_0$  is specific gas constant, V, Q, T are the velocity, heat flux, and temperature of the flow, respectively. The expression for  $f^{ma}$  is

$$f^{\mathrm{ma}}(\boldsymbol{x}, \boldsymbol{v}, t) = \frac{\rho}{(2\pi\mathsf{R}_0 T)^{3/2}} \exp\left(-\frac{\boldsymbol{c}^2}{2\mathsf{R}_0 T}\right), \qquad (5)$$

where  $\rho$  is density of gas.

Using the Shakhov model, Eqn. (1) is simplified to

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_x f = \frac{1}{\tau} (f^{\rm sh} - f). \tag{6}$$

DVM uses discretized values of f over both the physical domain and the velocity domain to solve Eqn. (6) numerically. Let  $\{\hat{v}_1, \hat{v}_2, \dots, \hat{v}_{N_v}\}$  be a set of  $N_v$  fixed velocity points, Eqn. (6) is discretized in velocity domain as

$$\frac{\partial \hat{f}_k}{\partial t} + \hat{v}_k \cdot \nabla_x \hat{f}_k = \frac{1}{\tau} (\hat{f}_k^{\rm sh} - \hat{f}_k) \tag{7}$$

for  $1 \leq k \leq N_v$ , where  $\hat{f}_k^{\rm sh}$  stands for  $f^{\rm sh}(\boldsymbol{x}, \hat{v}_k, t)$  and  $\hat{f}_k$ stands for  $f(\boldsymbol{x}, \hat{v}_k, t)$ . Note that, if the RHS of Eqn. (7) is treated as an external source, Eqn. (7) represents a system of convection equations, each with fixed velocity  $\hat{v}_k$ . The system of convection equations can be solved efficiently via many of the established methods in computational fluid mechanics. In this paper, we use the same finite volume method (FVM) spatial discretization for all the  $N_k$  equations.

#### 2.2.1. Macroscopic quantities

For computation of  $f^{\text{sh}}$  and for evaluation of the flow field, macroscopic quantities such as density, velocity, temperature, etc. are usually required. These quantities can be obtained as moments of the distribution function f.

$$\rho(\boldsymbol{x},t) = \int_{\mathbf{R}^3} f(\boldsymbol{x},\boldsymbol{v},t) d\boldsymbol{v},\tag{8}$$

$$\boldsymbol{V}(\boldsymbol{x},t) = \frac{1}{\rho} \int_{\mathbf{R}^3} f(\boldsymbol{x},\boldsymbol{v},t) \boldsymbol{v} d\boldsymbol{v}, \tag{9}$$

$$p(\boldsymbol{x},t) = \frac{1}{3} \int_{\mathbf{R}^3} f(\boldsymbol{x},\boldsymbol{v},t) (\boldsymbol{v}-\boldsymbol{V})^2 d\boldsymbol{v}, \qquad (10)$$

$$\boldsymbol{Q}(\boldsymbol{x},t) = \frac{1}{2} \int_{\mathbf{R}^3} f(\boldsymbol{x},\boldsymbol{v},t) (\boldsymbol{v}-\boldsymbol{V}) (\boldsymbol{v}-\boldsymbol{V})^2 d\boldsymbol{v}.$$
(11)

In DVM, the integrals in Eqn. (8) to Eqn. (11) should be replaced by numerical quadrature. In this paper, 24-point and 50-point Gauss-Hermite quadrature are used. Temperature can be obtained by the equation of state

$$T = \frac{p}{\rho \mathsf{R}_0},\tag{12}$$

and relaxation time can be obtained by

$$\tau = \frac{\mu}{p} = \frac{\mu_0 (T/T_0)^{\omega}}{p},$$
(13)

where  $\mu_0$  is a reference value of  $\mu$  at temperature  $T_0$ , and  $\omega$  is a gas-specific constant. Once the macroscopic quantities are obtained,  $f^{\rm sh}$  can be explicitly calculated.

# 2.2.2. Boundary condition

For a computational domain C of rarefield flow, its boundary can be divided into two types: open and closed. Open boundaries are those where fluid is present on both sides, such as flow inlets/outlets, and far-field flows. For open boundaries, boundary conditions can be determined according to established results in CFD. For closed boundaries, gas molecules are reflected on the solid surfaces. The exact boundary conditions are given in terms of reflection kernels  $R_{\rm rfl}(\mathbf{v}_i, \mathbf{v}_r)$ , which states the probability density of a molecule getting reflected to velocity  $\mathbf{v}_r$  when it hits the surface with velocity  $\mathbf{v}_i$ . In DVM computation, solid boundaries are treated as extra source (or sink) of f.

### 2.2.3. Time marching scheme

In rarefied gas flows, turbulence is hardly present, and the focus is mainly on the steady state flow field. Therefore, an LUSGS-based implicit time marching scheme, as is described in reference<sup>(18)</sup> is used, which drastically speeds up convergence.

# Topology optimization and material interpolation Topology optimization

In topology optimization, we consider the problem to find the optimal structure that minimizes/maximizes a given objective function. The key idea is to replace the structure optimization problem by a material distribution problem, namely, for a characteristic function  $\chi$ , we let

$$\chi(\boldsymbol{x}) = \begin{cases} 1 & \boldsymbol{x} \in \mathcal{F}, \\ 0 & \boldsymbol{x} \in \mathcal{D} \backslash \mathcal{F}, \end{cases}$$
(14)

where  $\mathcal{D}$  is the design domain, and  $\mathcal{F}$  is fluid domain. However, as  $\chi$  can take either 1 or 0 for  $\boldsymbol{x} \in \mathcal{D}$ , infinitely small structures are not prohibited, resulting the optimization problem being ill-posed. One solution is to use a normalized density  $\alpha$  instead of  $\chi$  as the design variable, where  $\alpha$  is in  $\mathcal{L}^{\infty}(\mathcal{D}; [0, 1])$ , Lebesgue integrable functions defined over  $\mathcal{D}$ with value between 0 and 1. Using the pseudo design density can increase the regularity of the obtained structures<sup>(19)</sup>. However, introduction of  $\alpha$  brings a new problem. As  $\alpha$  can take values between 0 and 1, some intermediate state between solid and fluid is introduced. Therefore, the computational domain, which consists of pure fluid initially, will have to be extended to a domain of mixed fluid and solid.

#### 3.2. Material interpolation in DVM

In reference<sup>(14)</sup>, extension of the rarefied flow is achieved by extension of the Boltzmann equation. It is noted that the fixed solid can be treated as some porous media with varying permeability. A numerical scheme is then developed to solve the extended Boltzmann equation.

In this paper, we consider a more straightforward approach, where we directly construct an extension to the conventional DVM algorithm. Following the FVM spatial discretization, we let  $\vec{\alpha}$  denote the discretized representation of design variable  $\alpha$  in  $N_c$  computational cells. Namely,  $\vec{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_{N_c})'$ , where  $(\cdot)'$  denotes transposition. We state that the following properties should be satisfied by the extension:

- The result of extended DVM calculation should change continuously with  $\vec{\alpha}$ .
- For a given  $\vec{\alpha}$  whose elements are either 0 and 1, result of the extended DVM shall be the same as conventional DVM, where the computational domain is set to the union of all cells where  $\alpha = 1$ , and identical boundary conditions are applied.

Shifting the focus from the Boltzmann equation to DVM bypasses the cumbersome derivation processes, and allows us to control or fine-tune the material interpolation scheme directly. In the following subsections, we present the detailed description of our extended DVM scheme.

#### 3.2.1. Modification in convection flux

The DVM discretization transforms the Boltzmann equation into a system of convection equations (7). Using FVM spatial discretization to solve the convection equations involves evaluating the surface fluxes at the boundaries of the computational cells. Without loss of generality, we write the flux as  $\phi_k$  for the convection equation featuring  $\hat{v}_k$ . The detailed expression of  $\phi_k$  shall depend on the flux reconstruction scheme one chooses, for instance, first-order upwind, Van-Leer, essentially non-oscillation (ENO), etc. In conventional DVM, the computational domain consists purely of fluid, hence  $\phi_k$  that leaves the upwind cell flows entirely into the downwind cell. This ensures conservation of the FVM scheme. However, the the extension of DVM, our computational domain may include a mixture of different materials, as is indicated by the value of  $\alpha$  stored in each computational cell. In order to model the transfer from fluid ( $\alpha = 1$ ) to solid ( $\alpha = 0$ ), we suggest the following correction of convection flux, using the value of  $\alpha$  across the cell boundary. Still, we let  $\phi_k$  represent the flux obtained according to standard DVM,  $\alpha_{up}$  be the value of  $\alpha$  in the upwind cell, and  $\alpha_{down}$  be the value of  $\alpha$  in the downwind cell. The corrected scheme is described as follows.

- The flux that leaves the upwind cell becomes  $\alpha_{up}\phi_k$ .
- The flux that enters the downwind cell becomes  $\alpha_{up}\alpha_{down}\phi_k$ .
- In order to preserve conservation, the difference between the two fluxes,  $\alpha_{up}(1 - \alpha_{down})\phi_k$ , shall be fed to a local reflection kernel  $R_{rfl}^{local}$ , which describes postreflection conditions, if solid is present in the computational cell.

Note that, in this extended scheme, when  $\alpha_{up} = 0$ , the net flux that leaves the cell must be zero, which is in accordance with the idea that solid does not emit molecules into gas. On the other hand, when  $\alpha_{down} = 0$ , the flux enters the downwind cell must be zero, which means solid does not absorb molecules from gas. In that case,  $\alpha_{up} = \max(\alpha_{up} - \alpha_{down}, 0)$ , which means all the flux that leaves the upwind cells shall be reflected.

Also note that, the proposed scheme does not depend on the actual expressions of  $\phi_k$  and  $R_{\text{local}}$ , and only depends on  $\alpha_{\text{up}}$  and  $\alpha_{\text{down}}$ . This ensures the versatility, namely, this extension in convection flux can be applied to any flux reconstruction scheme and any reflection boundary condition.

# 3.2.2. Modification in relaxation time

In DVM, we use implicit time scheme to update the flow field. According to reference  $^{(18)}$ , the convection fluxes, as well as the  $-\frac{1}{\tau}f$  term on the RHS of Eqn. (3) are treated implicitly, while the Shakhov state  $\frac{1}{2}f^{sh}$  is treated as a constant source term in every iteration. This is because  $f^{\rm sh}$  depends on all the velocity components in one computational cell. If a full implicit scheme is used,  $f^{\rm sh}$  will have to be re-calculated after the update of every single velocity component, which is too expensive in computational terms. It can be shown that, when Kn is sufficiently large (Kn > 1), treating  $\frac{1}{\tau} f^{\rm sh}$  explicitly will not slow down convergence significantly, as convection still dominates the development of flow field. However, in the extended DVM scheme,  $\alpha$  restricts the effective convective fluxes between computational cells. As a result, when  $\alpha$  takes a non-zero small value, the magnitude of convective change will likely be overshadowed by the magnitude of relaxation change, which can be thought of as a local drop in Kn for the computational cell. Consequently, explicit treatment of  $\frac{1}{\tau}f^{\rm sh}$  cannot effectively update the flow field, and the speed of convergence could be drastically impaired.

In order to fix this local decrease in Kn and restore the computational efficiency, we suggest the relaxation term strength to be equally scaled by local value of  $\alpha$ . Namely, the collision integral W shall be modelled by

$$W[f] = \frac{\alpha}{\tau} (f^{\rm sh} - f). \tag{15}$$

Using the modified relaxation model ensures that the magnitude of convection and relaxation remain balanced according to a global Kn, so that the rate of convergence of the extended DVM will be at the same level compared to conventional DVM.

It may cause some confusion that for  $\alpha = 0$ , the relaxation term vanishes for solid regions, which is opposite to the model in reference (14), where solid is treated as regions where inter-molecular collisions are extremely strong. Note that, in our proposed method, despite relaxation is effectively non-existent for solid, the velocity distribution in solid region has zero effect on its neighbouring cells due to the correction in convection fluxes. The presence of solid (or cells where  $\alpha = 0$  is manifested by the additional reflection fluxes created at the cell boundaries, whose intensity depends entirely on the incident flux from outside the solid region. And since the effective convection flux from the upwind cell to the downwind is corrected by a factor  $\alpha_{up}\alpha_{down}$ , the influence of a computational cell to the entire computational domain is limited by the local value of  $\alpha$ . Together with modification of macroscopic flow quantities in the objective function, which will be introduced below, modifying  $\tau$  according to  $\alpha$  will not cause ill effects to the global flow field, even if  $0 < \alpha < 1$ .

## 3.2.3. Modification in objective function

In order to increase the convexity of the optimization problem, we suggest to add a penalty term in the final results of DVM calculation. Let  $\hat{\rho}, \hat{V}, \hat{p}, \hat{Q}$  be the density, velocity, pressure, and heat flux calculated from numerical quadrature, as is done in convectional DVM. In the extended DVM, we suggest using  $\hat{\rho^*}, \hat{V^*}, \hat{p^*}, \hat{Q^*}$  as substitutions. The definitions are

$$\hat{\rho^*} = \alpha^\beta \hat{\rho} + (1 - \alpha^\beta) \rho_0, \qquad (16)$$

$$\hat{V}^* = \alpha^\beta \hat{v} + (1 - \alpha^\beta) V_0, \qquad (17)$$

$$\hat{p^*} = \alpha^\beta \hat{p} + (1 - \alpha^\beta) p_0, \qquad (18)$$

$$\hat{Q^*} = \alpha^\beta \hat{Q} + (1 - \alpha^\beta) \boldsymbol{Q}_0, \qquad (19)$$

where  $\rho_0$ ,  $V_0$ ,  $p_0$ ,  $Q_0$  are constant values, representing the desired density, velocity, pressure, and heat flux of the flow field when solid is present. For steady solid,  $V_0 = Q_0 = 0$ . Gas density and pressure are not properly defined for a pure solid region, we suggest using the initial values in DVM calculation  $\rho_0 = \rho_{\text{ini}}$ ,  $p_0 = p_{\text{ini}}$ . The exponent  $\beta \ge 0$  controls the level of penalization.

#### 4. Sensitivity analysis via discrete adjoint system

In topology optimization, the key step, sensitivity analysis, is dedicated to evaluate the change of the objective functional due to changes in the design variable. The conventional sensitivity analysis approach is to use the Lagrangian multiplier method with adjoint variables. Like is done in ref $erence^{(14)}$ , a system of adjoint equations, with proper boundary conditions, should be derived based on the Boltzmann equation. After that, a separate numerical scheme is developed to solve for the adjoint variables numerically. This optimize-then-discretize (OTD) approach, as is discussed in reference (15), requires rigorous yet tedious derivations, which is particularly the case for the Boltzmann equation. In refer $ence^{(16)}$ , an alternative discretize-then-optimize (DTO) approach is used, where the focus is shifted to the numerical variables. The DTO approach by passes the derivation, and simplifies the formulation significantly. However, simply tracking the dependencies of the numerical variables from their initial values to the steady state solution incurs seriously high memory usage and lacks computational efficiency. In the following subsections, we shall introduce a discrete adjoint system based on the discretized version of the Boltzmann equation through the proposed extension of DVM.

#### 4.1. Symbolic expressions for the extended DVM

In extended DVM, we can write the discrete values  $\hat{f}_k$  in one state vector  $\vec{f} \in \mathbb{R}^{N_c N_v}$  ,

$$\vec{f} = (\vec{f}_1, \vec{f}_2, \cdots, \vec{f}_{N_c})',$$
 (20)

where each  $\vec{f}_i \in \mathbb{R}^{N_v}$  represents the discretized  $\hat{f}_k (1 \leq k \leq N_v)$  in the computational cell indexed i,

$$\hat{f}_i = (\hat{f}_{1,i}, \hat{f}_{2,i}, \cdots, \hat{f}_{N_v,i})'.$$
 (21)

The extended DVM updates the state vector  $\vec{f}$  at every time step until the flow field reaches steady state. The steady state can be identified as the zero of a residual operator  $\vec{R}(\vec{f}) \in \mathbb{R}^{N_c N_v}$ .  $\vec{R}$  takes the current discretized value  $\vec{f}$  as input, and returns the rate of change with respect to time for every component. The detailed expressions of  $\vec{R}$  should depend on the FVM discretization of the computational domain, the flux reconstruction scheme for the convection equations, and  $\vec{\alpha}$ . Therefore, the steady state of the rarefied flow field, as is dictated by

$$\boldsymbol{v} \cdot \nabla_x \boldsymbol{f} = \boldsymbol{W}[\boldsymbol{f}] \tag{22}$$

can be rewritten in discrete form as

$$\vec{R}(\vec{f};\vec{\alpha}) = 0. \tag{23}$$

Note that, the boundary conditions of Eqn. (22) are automatically included in Eqn. (23) by proper definition of  $\vec{R}$ .

#### 4.2. Discrete optimization problem

Following the discretized governing equation, we consider the model optimization problem for rarefied flow field.

$$\inf_{\vec{\alpha}} K = K(f; \vec{\alpha}), \tag{24}$$

subject to

$$\vec{R}(\vec{f};\vec{\alpha}) = 0. \tag{25}$$

K is a objective functional to be minimized, and is defined over the state vector  $\vec{f}$  and the pseudo design density  $\vec{\alpha}$ . Note that the expression of K is very general, as all the macroscopic flow quantities can be obtained from the discrete velocity distribution function via proper quadrature. Equation (25) uses the discretized expression of steady state.

#### 4.3. Discrete adjoint system

Design sensitivity is obtained using the augmented Lagrangian multiplier method with adjoint variables. We define the Lagrangian J as

$$J = K(\vec{f}; \vec{\alpha}) - \vec{\Phi} \cdot \vec{R}(\vec{f}; \vec{\alpha})$$
<sup>(26)</sup>

In  $J, \vec{\Phi} \in \mathbb{R}^{N_c N_v}$  is the vector of adjoint variables. According to first-order optimal conditions, we derive the adjoint equations by stating  $\frac{\partial J}{\partial \vec{f}} = 0$ , namely,

$$\frac{\partial K}{\partial \vec{f}} - \left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)' \vec{\Phi} = 0.$$
(27)

Note that,  $\frac{\partial K}{\partial \vec{f}}$  is the gradient of K with respect to  $\vec{f}$ , which is a vector in  $\mathbb{R}^{N_c N_v}$ .  $\frac{\partial \vec{R}}{\partial \vec{f}}$  is the Jacobian of flow residual  $\vec{R}$ with respect to  $\vec{f}$ , which is an  $N_c N_v \times N_c N_v$  square matrix. For known  $\vec{f}$  and  $\vec{\alpha}$ ,  $\frac{\partial K}{\partial \vec{f}}$  and  $\frac{\partial \vec{R}}{\partial \vec{f}}$  can be explicitly formulated. Therefore, symbolically speaking, Eqn. (27) is simply a system of linear equations. Once  $\vec{\Phi}$  is numerically solved, the sensitivity  $\vec{H}$  is obtained by

$$\vec{H} = \frac{\partial J}{\partial \vec{\alpha}} = \frac{\partial K}{\partial \vec{\alpha}} - \left(\frac{\partial \vec{R}}{\partial \vec{\alpha}}\right)' \vec{\Phi}.$$
 (28)

Similar to Eqn. (27),  $\frac{\partial K}{\partial \vec{\alpha}}$  and  $\frac{\partial \vec{R}}{\partial \vec{\alpha}}$  are gradient and Jacobian which can be explicitly evaluated given  $\vec{f}$  and  $\vec{\alpha}$ .

# 4.4. The transposed flux Jacobian

The main challenge of sensitivity analysis lies in Eqn. (27), where we need to find the inverse of the transposed flux Jacobian  $\left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)'$ . Let  $\mathcal{B}$  denote the original flux Jacobian  $\frac{\partial \vec{R}}{\partial \vec{f}}$ . Note that, due to the structure of  $\vec{f}$ ,  $\mathcal{B}$  can be written in the form of a  $N_c \times N_c$  block matrix. Each block  $\mathsf{B}_{i,j}$  is a  $N_v \times N_v$  sub-matrix, which corresponds to the Jacobian of flow residual in cell j with respect to the state vector in cell *i*. Note that, due to the locality of the FVM discretization, most of  $B_{i,j}$  will be zero.  $B_{i,j}$  is non-zero only when i = j or when *i*, *j* are adjacent computational cells. Therefore, the transposed system  $\mathcal{B}'$  is also a sparse matrix, which can be solved using the LUSGS technique with similar efficiency.

#### 4.5. Discussion regarding the adjoint variables

The sensitivity obtained via the discrete adjoint system is closely related to one that obtained from a finite-difference approach. Consider the objective functional  $K(\vec{f}, \vec{\alpha})$ , we would like to obtain its rate of change with respect to perturbations in  $\vec{\alpha}$ , which is to consider the total derivative

$$\frac{dK}{d\vec{\alpha}} = \frac{\partial K}{\partial \vec{f}} \frac{\partial \vec{f}}{\partial \vec{\alpha}} + \frac{\partial K}{\partial \vec{\alpha}}.$$
(29)

For given objective functional K and known values of  $\vec{f}$  and  $\vec{\alpha}$ , the two gradients  $\frac{\partial K}{\partial \vec{f}}$  and  $\frac{\partial K}{\partial \vec{\alpha}}$  can be explicitly evaluated. However, the remaining term  $\frac{\partial \vec{f}}{\partial \vec{\alpha}}$ , is less obvious.  $\vec{f}$  and  $\vec{\alpha}$  are related by the state equation (25), which dictates that zero flow residual should be attained by  $\vec{f}$  under given  $\vec{\alpha}$ . Therefore, for a small change in  $\vec{\alpha}$  to  $\vec{\alpha} + \Delta \vec{\alpha}$ , the current steady state  $\vec{f}$  must change to  $\vec{f} + \Delta \vec{f}$ , such that their induced changes in  $\vec{R}$  cancel out. Namely,

$$\vec{R}(\vec{f} + \Delta \vec{f}; \vec{\alpha} + \Delta \vec{\alpha}) = \vec{R}(\vec{f}; \vec{\alpha}) + \frac{\partial \vec{R}}{\partial \vec{f}} \Delta \vec{f} + \frac{\partial \vec{R}}{\partial \vec{\alpha}} \Delta \vec{\alpha} + \mathcal{O}[(\max(||\Delta \vec{f}||, ||\Delta \vec{\alpha}||)] = 0.$$
(30)

Note that the original steady state satisfies  $\vec{R}(\vec{f}; \vec{\alpha}) = 0$ , neglecting higher order terms, we have

$$\frac{\partial \vec{f}}{\partial \vec{\alpha}} = -\left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)^{-1} \frac{\partial \vec{R}}{\partial \vec{\alpha}}.$$
(31)

Substituting Eqn. (31) into Eqn. (29), we get an alternative expression for sensitivity

$$\frac{dK}{d\vec{\alpha}} = -\frac{\partial K}{\partial \vec{f}} \left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)^{-1} \frac{\partial \vec{R}}{\partial \vec{\alpha}} + \frac{\partial K}{\partial \vec{\alpha}}.$$
 (32)

Note that, the inverse  $\left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)^{-1}$  is not necessarily sparse, and would take up too much memory to store when  $N_c N_v$  is large. One possible solution is to use an iterative approach to calculate the result of Eqn. (31). However, note that  $\frac{\partial \vec{R}}{\partial \vec{\alpha}}$ is an  $N_c N_v \times N_c$  matrix. When  $N_c$  is large, this approach is still considerably expensive compared to finding the steady state flow field in DVM. One more feasible approach is to evaluate  $\frac{\partial K}{\partial \vec{f}} \left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)^{-1}$  first. Note that the transpose rule states that

$$\left[\frac{\partial K}{\partial \vec{f}} \left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)^{-1}\right]' = \left[\left(\frac{\partial \vec{R}}{\partial \vec{f}}\right)^{-1}\right]' \left(\frac{\partial K}{\partial \vec{f}}\right)' \qquad (33)$$

The solution of Eqn. (33) is exactly the adjoint variables  $\vec{\Phi}$ .

#### 5. Numerical examples

#### 5.1. Material interpolation

We use the following flow fields to demonstrate the validity of the proposed material interpolation scheme.



(b) Extended case.

Fig. 1: Computational domain of the plane Fourier flow.

# 5.1.1. Plane Fourier flow

In plane Fourier flow, rarefied gas is placed between two infinitely large parallel plates. The plates are stationary, but kept at different temperatures. The lower plate has  $T_{\rm low} = 0.5$ , and the higher plate has  $T_{\rm high} = 1.5$ , which are non-dimensionalized against reference temperature  $T_0 = 273$ K. The separation between the plates is 1 m, which is also the characteristic length of the flow field. Diffuse reflection boundary conditions are set at the gas/solid interfaces. We choose Argon as the working gas, and consider cases where a uniform initial density  $\rho_0$  results in Kn = 10.0, 1.0, 0.1, respectively.

As a benchmark case, we first calculate the flow field using standard DVM procedure. Due to the symmetry of the problem, we use 100 uniform-spaced computational cells to discretize the domain. The velocity domain is normalized by the reference speed  $v_0 = \sqrt{2R_0T_0}$ , and discretized using 50



Fig. 2: Temperature distribution in the plane Fourier flow at different Kn.

Gauss-Hermite quadrature nodes in each spatial direction, resulting  $N_v = 2500$  for the 2D case. For the discretized convection equations, first-order upwind scheme is used to reconstruct the surface flux.

To test the proposed material interpolation scheme, we consider an extended computational domain, where the separation between plates is increased to 1.2 m, and the number of uniform computational cells is increased to 120. In order to maintain the characteristic length, the lower 1/6 of the computational domain is assigned  $\alpha = 0$ , and the rest 5/6 is assigned  $\alpha = 1$ . Illustration of the computational domains is included in Fig. 1. Fig. 2 and Fig. 3 show the distribution of temperature and heat flux (normalized against  $Q_0 = \rho_0 v_0^3$ ). In the flow region where  $\alpha = 1$ , the extended DVM gives identical results compared to the benchmark cases. In the extended region where  $\alpha = 0$ , due to the modification scheme introduced in Section 3.2.3, macroscopic quantities actually do not depend on DVM results. Flow temperature and heat flux are simply forced to be 1.0 and 0.0, respectively, which are prescribed values to represent the presence of solid. Of course, the choice of representation of solid is a rather arbitrary one, for instance, one can use 0.5 to represent solid temperature in this plane Fourier flow.



Fig. 3: Heat flux distribution in the plane Fourier flow at different Kn.

#### 5.1.2. Plane Couette flow

The setup of plane Couette flow is similar to that of the plane Fourier flow, as is shown in Fig. 4. Rarefied Argon is placed between two infinitely large parallel plates separated by 1 m. Both plates are kept at T = 1.0, but the upper plate moves at  $v_{\text{plate}} = 0.1$  (normalized against  $v_0$ ). The solid surfaces are treated as diffuse reflectors. We use the same discretization scheme as the Fourier flow, which is 50 Gauss-Hermite points in each spatial direction, and  $N_v = 2500$ . Three cases are considered where Kn = 10.0, 1.0, 0.1, respectively. Again, we consider a benchmark case and an extended case, where the separation is increased to 1.2 m, and the lower 1/6 of the computational domain is marked by  $\alpha = 0$ .



(b) Extended case.

Fig. 4: Computational domain of the plane Couette flow.

Fig. 5 and Fig. 6 show the distribution of x-velocity (normalized against  $v_0$ ) and shear stress (normalized against  $\rho_0 v_0^2$ ). Note that in the flow region where  $\alpha = 1$ , the extended DVM gives identical results compared to the benchmark cases. In regions where  $\alpha = 0$ , like the case of plane Fourier flow, the final velocity and shear stress are effectively independent of DVM results. Their values are both set to 0 due to the modification scheme in final macroscopic quantities.

#### 5.1.3. Cavity with inlet and outlet

We consider a 2D cavity with an inlet and an outlet, as is shown in Fig. 7. At the inlet, gas density and pressure are fixed at unit value. At the outlet, vacuum condition is imposed, which means no molecules can come in. Knudsen number is set to Kn = 1.0. The computational domain is divided into two regions  $C_1$  (white color) and  $C_2$  (gray color).



Fig. 5: x-velocity distribution in the plane Couette flow at different Kn.

In  $C_1$ , we set  $\alpha = 1$ . In  $C_2$ , we consider three cases where  $\alpha = 0, 0.5$  and 1. The distribution of flow velocity is shown in Fig. 10. It can be seen that as  $\alpha$  in  $C_2$  increases from 0 to 1, the velocity in  $C_2$  gradually increases, until it merges with  $C_1$  as a whole. The physical domain is discretized by  $100 \times 100$  uniform square cells, and the velocity domain is discretized by the same 2500 Gauss-Hermite points in 2D as in previous cases.

#### 5.2. Sensitivity from discrete adjoint system

We use the same 2D cavity problem to demonstrate the validity of design sensitivity obtained from the discrete adjoint system. The discretization schemes in both physical and velocity domains are kept identical. Consider the objective functional K defined as the flow rate at the inlet. Namely, K is the average of flow velocity in the x-direction at  $\Gamma_{\rm in}$ . In discrete terms, K is obtained by the average of



Fig.6: Shear stress distribution in the plane Couette flow at different Kn.

x-velocity among all the cells at  $\Gamma_{\rm in}$ , which are obtained according to Eqn. (17). We consider the case where  $\alpha = 1$  in the computational domain, which means the cavity is filled with rarefied gas. Letting  $\beta = 0$ , we can solve the adjoint equation for  $\Phi$ , and obtain  $\vec{H}$  in every computational cell. The results are shown in Fig. 8.

A comparison of  $\vec{H}$  with its finite difference counterpart  $\vec{H}_{\rm FD}$  is provided in Fig. 9, where the absolute value of the difference is shown. We can see that the results are in good agreement. The definition of the *i*-th element of  $\vec{H}_{\rm FD}$  is

$$H_{\mathrm{FD},i} = \frac{K(\vec{\alpha} + \epsilon \vec{e}_i) - K(\vec{\alpha})}{\epsilon}, \qquad (34)$$

where  $\vec{e}_i$  is the *i*-th unit vector, and  $\epsilon$  is a small value, chosen as  $10^{-4}$  in this example.  $\vec{H}_{\rm FD}$  can be interpreted as a finite difference approximation of the design sensitivity. It is simply the ratio between the change of objective functional



Fig. 7: Computational domain of the cavity flow.



Fig. 8: Sensitivity distribution in the computational domain



Fig. 9: Error distribution in the computational domain

K and the change in design variable  $\vec{\alpha}.$ 

# 6. Conclusion

In this research, material interpolation scheme and sensitivity analysis method is developed for topology optimization of rarefied gas flows. The main results are listed as follows.

- 1. Based on the DVM for rarefied gas flows, a material interpolation scheme is proposed, which allows parametrization of solid/fluid distribution in the design domain using a pseudo density. The proposed scheme can be applied for any reflection boundary condition, and does not impair the computational efficiency of standard DVM.
- 2. A discrete adjoint system is formulated based on functional representation of the extended DVM algorithm and the Lagrangian multiplier method. The adjoint system can be numerically solved by transposing the flux Jacobian.
- 3. The proposed interpolation scheme and sensitivity analysis method is validated by numerical examples.

The proposed method may serve as the basis for structural optimization of rarefied gas flows.

#### 参考文献

- Sharipov, F.: Rarefied gas dynamics: fundamentals for research and practice, (2015).
- (2) Takaishi, T and Sensui, Y.: Thermal transpiration effect of hydrogen, rare gases and methane, Transactions of the Faraday Society, 59(1963), pp. 2503–2514.
- (3) Aristov V.V., Shakhov E.M., Titarev V.A., and Zabelok S.A: Comparative study for rarefied gas flow into vacuum through a short circular pipe, Vacuum, 103 (2014), pp. 5–8.
- (4) Wang Y., Liu S., Zhuo C., and Zhong C.: Investigation of nonlinear squeeze-film damping involving rarefied gas effect in micro-electro-mechanical systems, Computers and Mathematics with Applications, 114(2022), pp. 188–209.
- (5) Oran, Elaine S., Oh, C.K. and Cybyk, B.Z.: Direct simulation Monte Carlo: recent advances and applications, Annual Review of Fluid Mechanics, **30**(1998), pp. 403– 441.
- (6) Alexander, Francis J. and Garcia, Alejandro L.: The direct simulation Monte Carlo method, Computers in Physics, 11(1997), pp. 588–593.
- Broadwell, James E.: Study of rarefied shear flow by the discrete velocity method, Journal of Fluid Mechanics, 19(1964), pp. 401–414.

- (8) Yang, LM, Shu, C., Yang, WM., Chen, Z., and Dong,
  H: An improved discrete velocity method (DVM) for efficient simulation of flows in all flow regimes, Physics of Fluids, **30**(2018)
- (9) Shokouhmand, H., Isfahani, AH Meghdadi: An improved thermal lattice Boltzmann model for rarefied gas flows in wide range of Knudsen number, International communications in heat and mass transfer, **38**(2011), pp. 1463–1469.
- (10) Zhang Y., Qin R., and Emerson, David R:Lattice Boltzmann simulation of rarefied gas flows in microchannels, Physical review E, **71**(2005), pp. 047702.
- (11) Hassan A., Ehsan R, and Stefan S.: A comprehensive review on micro- and nano-scale gas flow effects: Slip-jump phenomena, Knudsen paradox, thermallydriven flows, and Knudsen pumps, Physics Reports, **997**(2023), pp. 1–60.
- (12) Bond D.M., Wheatley V., and Goldsworthy M.: Numerical investigation into the performance of alternative Knudsen pump designs, International Journal of Heat and Mass Transfer, **93** (2016), pp. 1038–1058.
- (13) Kugimoto K., Hirota Y., Yamauchi T., Yamaguchi H. and Niimi T.: Design and demonstration of Knudsen heat pump without moving parts free from electricity, Applied Energy, **250**(2019), pp. 1260–1269.
- (14) Sato A., Yamada T., Izui K., Nishiwaki S., and Takata S.: A topology optimization method in rarefied gas flow problems using the Boltzmann equation Journal of Computational Physics, **395**(2019), pp. 60-84.
- (15) Caflisch R., Silantyev D., and Yang Y.: Adjoint DSMC for nonlinear Boltzmann equation constrained optimization, Journal of Computational Physics, 439(2021) pp. 110404.
- (16) Guan K., Matsushima K, Noguchi Y., and Yamada T.: Topology optimization for rarefied gas flow problems using density method and adjoint IP-DSMC, Journal of Computational Physics, 474(2023), pp. 111788.
- (17) Bird, G. A.: Molecular Gas Dynamics And The Direct Simulation Of Gas Flows, (1994).
- (18) Zhu L., Pi X., Su W., Li Z.H., Zhang Y., and Wu L.: General synthetic iterative scheme for nonlinear gas kinetic simulation of multi-scale rarefied gas flows, Journal of Computational Physics, **430** (2021) pp. 110091.
- (19) Bendsøe, M.P. and Sigmund, O.: Material interpolation schemes in topology optimization, Archive of Applied Mechanics, 69(1999) pp. 635–654.









Fig. 10: x-velocity distribution in the cavity when the bottom-left corner is filled with different  $\alpha_2$ .