

Computational Physics

An efficient solution algorithm for force-driven continuum and rarefied flows

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ABSTRACT

Gaseous flows under an external force are intrinsically defined by their multi-scale nature due to the large variation of densities along the forcing direction. Devising a numerical method capable of accurately and efficiently solving force-driven cross-scale flow dynamics, encompassing both continuum and rarefied regimes, continues to pose a formidable and enduring challenge. In this work, a novel solution algorithm for multi-scale and non-equilibrium flow transport under an external force is developed based on the Boltzmann-BGK equation. The core innovation lies in the fusion of the Hermite spectral method (employed to characterize non-equilibrium particle distributions) with a multi-scale evolution model (sourced from the unified gas-kinetic scheme), achieving a seamless connection between computational methods and physical models. To accommodate the properties of the spectral-collocation method, a series of collocation points and weights are adapted based on the Gauss-Hermite quadrature. As a result, the computational efficiency of the solution algorithm is significantly improved (up to 50 times) while maintaining comparable accuracy as the classical discrete velocity method. It is demonstrated that the solution algorithm effectively preserves the key structural features of gas-dynamic systems subjected to an external force, e.g., the well-balanced property. Extensive numerical experiments have been performed to verify the accuracy and efficiency of the proposed method, including the one-dimensional hydrostatic equilibrium problem, the Sod shock tube, the Fourier flow, the Poiseuille flow, and the Rayleigh-Taylor instability problem. The proposed methodology can provide substantive theoretical insights into a wide range of engineering challenges involving force-driven multi-scale flows. The open-source codes to reproduce the numerical results are available under the MIT license <https://github.com/CFDML/Hermite-UGKS>.

1. Introduction

Classical gas dynamics is established based on corresponding characteristic scales. At the spatial and temporal scales of molecular mean free path and collision time, the Boltzmann equation is established to statistically describe the transport of a vast ensemble of particles, thereby depicting fluid motions at the kinetic scale. At a macroscopic level, the Navier-Stokes equations are used to characterize the collective behaviors of particle transport, e.g., phenomena involving wave propagation and interaction. Scale separation provides the foundation for the applicability of different models, especially for shifting from intricate molecular descriptions to manageable continuum models. Numerical methods for computational fluid dynamics have been developed for solving the governing equations at different scales, e.g., the discrete velocity method for the Boltzmann equation [1] and the Riemann-problem-based flux solver for compressible Navier-Stokes equations [2].

The principle of scale separation is not universally applicable. An easily overlooked example is gaseous flows under external force. It can be theoretically demonstrated that the density and pressure of gases are exponentially distributed under a unidirectional constant external force [3]. The exponential factor manifests as ah/RT , with a being the magnitude of forcing acceleration, h the length of the domain, T the temperature, and R the gas constant. In an ordinary laboratory environment, the factor is moderate, and thus, classical gas dynamics routinely ignores the effects of external force. As we focus on large-scale flows, e.g., atmospheric circulation, the influence exerted by the external force cannot be disregarded. Comparable scenarios may occur at small scales accompanied by large accelerations, e.g., Vlasov-type forces in plasmas and dense gases [4]. Note that the acceleration of a non-inertial frame also gives rise to fictitious forces, e.g., centrifugal and Coriolis forces. The study of gas dynamics under an external force is both a fascinating research pursuit and of notable engineering significance.

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Table 1
Nomenclature.

t	time variable
$\mathbf{x}$	space variable (x, y, z)
$\mathbf{v}$	velocity variable (u, v, w)
$\mathbf{a}$	external force acceleration
f	particle distribution function
$\mathcal{Q}$	collision operator in kinetic equation
$\mathcal{M}$	Maxwellian distribution function
ν	relaxation frequency
τ	relaxation time ($\tau = 1/\nu$)
μ	dynamic viscosity
p	pressure
m	molecular mass
k	Boltzmann constant
ρ	macroscopic density
$\mathbf{V}$	macroscopic velocity
T	macroscopic temperature
E	macroscopic energy
ψ	collision invariants
$\mathbf{W}$	macroscopic conservative variables ($\rho, \rho\mathbf{V}, \rho E$)
$\mathbf{P}$	stress tensor
$\mathbf{q}$	heat flux
Ω	computational domain
V	volume of domain
$\mathbf{F}^f$	numerical flux for distribution function
$\mathbf{F}^W$	numerical flux for conservative variables
$\mathbf{S}$	area vector of cell face
$\bar{G}$	source term for distribution function
$\mathbf{G}$	source term for conservative variables
σ	reconstructed spatial slope of distribution function
θ	spatial slope of equilibrium distribution function
ϕ	temporal slope of equilibrium distribution function
$\bar{m}$	equilibrium flux contribution
$\bar{f}$	initial flux contribution
H	generalized Heaviside function
$\mathcal{H}$	Hermite polynomials
$\mathbf{u}$	rescaled particle velocity
$\mathbf{d}$	expansion coefficients
ω	weight function in the Hermite expansion
δ	identity tensor
$\mathbf{T}$	modified stress tensor
$\mathbf{Q}$	modified heat flux tensor

Differences in gas density along the forcing direction result in varying characteristic scales of flows. Employing the Knudsen number (i.e., the ratio of the molecular mean free path to a length scale of interest) as the criterion, flows within spatially distinct regions can be categorized into different regimes [5]. The Navier-Stokes equations, formulated in the continuum regime, prove inadequate for the precise description of rarefied flows. This inapplicability is even more pronounced under an external force. In the Navier-Stokes equations, the external force appears only as a source term for the velocity field. I.e., it contributes solely to the kinematics and does not alter the dynamics of the fluid system. Asymptotic analysis of the Boltzmann equation shows that external force can induce the generation of non-equilibrium stress and heat flux [6,7]. This phenomenon arises due to the asymmetric tendency of particle transport caused by acceleration and is therefore observable under a non-vanishing mean free path (e.g., in the Navier-Stokes regime). Fine-grained mesoscopic modeling and simulation are essential to accurately capture non-equilibrium transport phenomena under external forces.

A wealth of numerical methods has been advanced to address non-equilibrium flows, with the stochastic particle method and the discrete velocity method for the Boltzmann equation standing as two of the most prominent approaches. By integrating coupled transport and collision processes in the particle evolution model and developing implicit and semi-implicit update algorithms, these methodologies can be extended to encompass cross-scale flow simulations. Among others, exemplary achievements include asymptotic preservation methods [8–10], high-order/low-order algorithms [11], gas-kinetic schemes [12–14], iterative schemes [15], multi-scale particle methods [16–19]. However, the pres-

ence of external forces places additional demands on the performance of numerical methods. Under a unidirectional constant force, a gas dynamic system will evolve toward and persist with a steady state with zero macroscopic velocity from an arbitrary initial state. Such hydrostatic equilibrium should be maintained by realizing an exact balance between the force term and the inhomogeneous flux function in the numerical method. The lack of such a well-balanced property leads to spurious numerical solutions, especially in long-time self-evolving gravitational systems.

Current research on well-balanced methods predominantly centers on hyperbolic conservation laws [20–23], while limited attention has been devoted to rarefied and multi-scale flows. Developing well-balanced methods for macroscopic and kinetic equations fundamentally constitutes different challenges. In the continuum limit, it can be deduced that in hydrostatic equilibrium the gas dynamic system has the same temperature everywhere [24]. However, as the local Knudsen number increases, the force-induced heat fluxes lead to a heterogeneous temperature distribution. At this juncture, the temperature can no longer be routinely treated as a constant multiplier. Instead, it must be incorporated into the evolving framework of the gas dynamic model. The unified gas-kinetic scheme (UGKS) provides such a model, where the characteristic lines of the Bhatnagar-Gross-Krook model [25] (as a simplified model of the Boltzmann equation) that contain particle trajectory information, can be introduced in the construction of numerical fluxes. Based on the UGKS, well-balanced methods have been developed for single- and multi-component gas transport [26,27]. Other pioneering work on multi-scale methods for the flows under an external force can be found in the literature [28,29].

Among other discrete velocity methods, the UGKS employs a uniform nodal description in the physical-velocity phase space. The well-balanced property is satisfied in an asymptotic basis as the number of collocation points $N_c \rightarrow 0$. However, in real numerical simulations, the number of discrete meshes is always finite. The preservation of physical structure only holds practical significance when discussed in conjunction with aliasing, interpolation, and integral errors. A prime illustration lies in the fact that particle methods, while fundamentally grounded in first-principles modeling, are rendered impractical for the development of well-balanced methods due to statistical errors. The existence of an external force field necessitates solving the derivative of particle distributions in the velocity space. A straightforward finite difference approximation leads to an error of $O(\Delta v)$ where $v \in (-\infty, \infty)^3$. Since the number of velocity collocation points is usually smaller than the number of elements in the physical space, such an error is considerably substantial.

Spectral methods offer an accurate approach for approximating solutions to differential equations. By approximating the solution as a sum of basis functions, the error can decrease exponentially with the number of bases, and fewer degrees of freedom are usually required to obtain comparable solutions from the finite difference method. Hermite polynomials prove exceptionally advantageous for approximating distribution functions in the Boltzmann equation, owing to the orthogonality with respect to Gaussian weighting functions, which corresponds to the Maxwellian equilibrium distribution. Such orthogonality warrants that the deviation from equilibrium can be accurately represented and efficiently decomposed into physically meaningful moment variables. It has been shown that the Hermite polynomials can asymptotically converge to non-equilibrium distribution functions [30]. In this study, we present a unified Galerkin-collocation method for multi-scale flows under external force by synergistically integrating the Hermite spectral method with the multiscale evolutionary model, i.e., the UGKS. By employing the spectral and collocation methods to compute the forcing and advection terms of the Boltzmann model equation, respectively, the solution algorithm is anticipated to harmonize accuracy with the capability to provide highly non-equilibrium and discontinuous solutions. A series of collocation points and weights applicable to the solution algorithm are adapted based on the Gauss-Hermite quadrature.

The rest of this paper is organized as follows. Section 2 briefly introduces the kinetic theory of gases under an external force. Section 3 provides the implementation of the solution algorithm and the corresponding numerical analysis. Section 4 includes numerical experiments to demonstrate the performance of the proposed approach, followed by the conclusions. The nomenclature of this paper is provided in Table 1.

2. Kinetic theory

The Boltzmann equation in the presence of an external force writes

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = Q(f), \quad (1)$$

where $f(t, \mathbf{x}, \mathbf{v})$ is the particle distribution function in the phase space, $\mathbf{v}$ is the particle velocity, $\mathbf{a}$ is the forcing acceleration, and Q is the intermolecular collision term. The full Boltzmann collision term is a nonlinear fivefold integral. Simplified models, e.g., the BGK model, are often adopted in engineering analysis and simulation to reduce the computational overhead. In the BGK model, the collision term is replaced by a relaxation operator, i.e.,

$$Q(f) = \nu(\mathcal{M} - f), \quad (2)$$

where ν is the relaxation frequency, and $\mathcal{M}$ denotes the Maxwellian distribution,

$$\mathcal{M} = \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{m}{2kT} (\mathbf{v} - \mathbf{V})^2\right), \quad (3)$$

where m is the molecular mass, k is the Boltzmann constant, $\{\rho, \mathbf{V}, T\}$ are the macroscopic density, velocity, and temperature, respectively.

Microscopic and macroscopic states are interconnected. The macroscopic conservative variables in fluid mechanics can be obtained by taking moments of the particle distribution function, i.e.,

$$\mathbf{W}(t, \mathbf{x}) = \begin{pmatrix} \rho \\ \rho \mathbf{V} \\ \rho E \end{pmatrix} = \int_{\mathbb{R}^3} f \psi d\mathbf{v}, \quad (4)$$

where $\psi = (1, \mathbf{v}, \mathbf{v}^2/2)^T$ is the vector of collision invariants that satisfies

$$\int_{\mathbb{R}^3} Q(f) \psi d\mathbf{v} = 0. \quad (5)$$

The transport equations of conservative variables can thus be obtained, i.e.,

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{V}) &= 0, \\ \frac{\partial \rho \mathbf{V}}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{V} \otimes \mathbf{V}) + \nabla_{\mathbf{x}} \cdot \mathbf{P} &= \rho \mathbf{a}, \\ \frac{\partial \rho E}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho E \mathbf{V}) + \nabla_{\mathbf{x}} \cdot (\mathbf{P} \cdot \mathbf{V}) + \nabla_{\mathbf{x}} \cdot \mathbf{q} &= \rho \mathbf{V} \cdot \mathbf{a}, \end{aligned} \quad (6)$$

where $\otimes$ denotes the dyadic product operator, and the stress tensor $\mathbf{P}$ and heat flux $\mathbf{q}$ are defined as

$$\mathbf{P} = \int_{\mathbb{R}^3} (\mathbf{v} - \mathbf{V}) \otimes (\mathbf{v} - \mathbf{V}) f d\mathbf{v}, \quad \mathbf{q} = \int_{\mathbb{R}^3} \frac{1}{2} (\mathbf{v} - \mathbf{V})(\mathbf{v} - \mathbf{V})^2 f d\mathbf{v}. \quad (7)$$

Note that the derivation from Eqs. (1) to (6) introduces no assumptions before incorporating a closure model, e.g., the Chapman-Enskog expansion.

3. Solution algorithm

3.1. Update algorithm

The solution algorithm is built upon the finite volume method. The computational domain is divided into N_x non-overlapping cells, i.e.,

$$\Omega = \bigcup_{i=1}^{N_x} \Omega_i, \quad \bigcap_{i=1}^{N_x} \Omega_i = \emptyset. \quad (8)$$

In each cell, the particle distribution function is approximated using collocation points N_v . The update algorithm of the cell-averaged particle distribution function can be written as

$$\begin{aligned} \frac{\partial f_{i,j}}{\partial t} &= -\frac{1}{V_i} \oint_{\partial \Omega_i} \mathbf{F}_j^f(t, \mathbf{x}) \cdot d\mathbf{S} + G(f_{i,j}) + Q(f_{i,j}) \\ &= -\frac{1}{V_i} \sum_{k=1}^{N_f} \mathbf{F}_{k,j}^f \cdot \Delta \mathbf{S}_k - \mathbf{a} \cdot \nabla_{\mathbf{v}_j} f_{i,j} + \nu_i (\mathcal{M}_{i,j} - f_{i,j}), \end{aligned} \quad (9)$$

where $f_{i,j}$ represents the averaged distribution function at the j th collocation point in the i th cell, V_i denotes the cell volume, $\mathbf{F}^f$ is the numerical flux of the distribution function, $\mathbf{S} = \mathbf{n} \Delta \mathbf{S}$ is the area vector pointing out of the cell, N_f is the number of faces, and G is the external force term.

Following the derivation of Eq. (6), taking moments of Eq. (9) over velocity space yields the semi-discrete conservation laws, i.e.,

$$\frac{\partial \mathbf{W}_i}{\partial t} = -\frac{1}{V_i} \oint_{\partial \Omega_i} \mathbf{F}_i^W \cdot d\mathbf{S} + \mathbf{G}_i = -\frac{1}{V_i} \sum_{k=1}^{N_f} \mathbf{F}_k^W \cdot \Delta \mathbf{S}_k + \mathbf{G}_i, \quad (10)$$

where the source term related to the external force is $\mathbf{G} = (0, \rho \mathbf{a}, \rho \mathbf{V} \cdot \mathbf{a})^T$. The cell-averaged conservative variables in Ω_i can be approximated by numerical quadrature at the discrete level, i.e.,

$$\mathbf{W}_i = \int_{\mathbb{R}^3} f_i \psi d\mathbf{v} \approx \sum_{j=1}^{N_v} w_j f_{i,j} \psi_j, \quad (11)$$

where w_j denotes the quadrature weights. Within the allowable range of integral errors, the update of macroscopic flow variables is equivalent to that of the particle distribution function. However, due to the absence of a source term in Eq. (10), the nested updating of macroscopic variables and the distribution function leads to gains in the numerical solution. For example, the updated macroscopic variables can be used to evaluate the equilibrium distribution function in Eq. (2) and subsequently solve Eq. (9). Such an implicit-explicit (IMEX) scheme is capable of mitigating the stiffness of the kinetic equation in the continuum limit. In this paper, the macroscopic conservative variables and the particle distribution function are updated simultaneously.

In this study, the IMEX scheme is routinely used to integrate Eq. (9) in a single time step Δt . Specifically, the collision term is solved implicitly for the sake of numerical stability, while the flux and source terms related to external forces are treated explicitly. The update algorithm writes

$$\frac{f_{i,j}^{n+1} - f_{i,j}^n}{\Delta t} = -\frac{1}{V_i} \sum_{k=1}^{N_f} \mathbf{F}_{k,j}^f \cdot \Delta \mathbf{S}_k - \mathbf{a} \cdot \nabla_{\mathbf{v}_j} f_{i,j}^n + \nu_i (\mathcal{M}_{i,j}^{n+1} - f_{i,j}^{n+1}), \quad (12)$$

which can be reformulated as

$$f_{i,j}^{n+1} = \left(\frac{1}{1 + \nu_i \Delta t} \right) \left(f_{i,j}^n - \frac{\Delta t}{V_i} \sum_{k=1}^{N_f} \mathbf{F}_{k,j}^f \cdot \Delta \mathbf{S}_k - \Delta t \mathbf{a} \cdot \nabla_{\mathbf{v}_j} f_{i,j}^n + \Delta t \nu_i \mathcal{M}_{i,j}^{n+1} \right). \quad (13)$$

To obtain the equilibrium information $\mathcal{M}^{n+1}$ in Eq. (13), the conservative variables are updated first, i.e.,

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n - \frac{\Delta t}{V_i} \sum_{k=1}^{N_f} \mathbf{F}_k^W \cdot \Delta \mathbf{S}_k + \Delta t \mathbf{G}_i. \quad (14)$$

The obtained macroscopic variables $\mathbf{W}^{n+1}$ can then be used to determine the equilibrium distribution function $\mathcal{M}^{n+1}$.

3.2. Numerical flux

The core task of the finite volume method is the computation of numerical fluxes. In this study, we employ the integral solution of the BGK equation to formulate the flux function. This practice has gained widespread acceptance in a series of gas-kinetic schemes to construct

multi-scale numerical methods [31]. If we assume the relaxation frequency to be a local constant, Eq. (2) yields an integral solution in the form

$$f(t, \mathbf{x}, \mathbf{v}) = \frac{1}{\tau} \int_0^t \mathcal{M}(t', \mathbf{x}', \mathbf{v}') e^{-(t-t')/\tau} dt' + e^{-(t-t^0)/\tau} f(t^0, \mathbf{x}^0, \mathbf{v}^0), \quad (15)$$

where $\tau = 1/\nu$ is the particle collision time, $\mathbf{x}' = \mathbf{x} - \mathbf{v}'(t - t') - \frac{1}{2}\mathbf{a}(t - t')^2$ and $\mathbf{v}' = \mathbf{v} - \mathbf{a}(t - t')$ are the particle trajectories in physical and velocity space, and $\{\mathbf{x}^0 = \mathbf{x} - \mathbf{v}^0(t - t^0) - \frac{1}{2}\mathbf{a}(t - t^0)^2, \mathbf{v}^0 = \mathbf{v} - \mathbf{a}(t - t^0)\}$ are the initial locations in phase space.

We then construct the numerical fluxes by approximating the equilibrium and initial distributions in Eq. (15), respectively. For brevity, we denote a face located between cells i and $i + 1$ as $\mathbf{x}_{i+1/2} = 0$, and the n th time step as $t^n = 0$. Eq. (15) can be rewritten in the discrete velocity coordinates as

$$f(t, 0, \mathbf{v}_j) = \frac{1}{\tau} \int_0^t \mathcal{M}(t', \mathbf{x}', \mathbf{v}'_j) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f(0, \mathbf{x}^0, \mathbf{v}^0_j). \quad (16)$$

This initial particle distribution function is constructed as

$$f(0, \mathbf{x}, \mathbf{v}_j) = f_0(\mathbf{x}, \mathbf{v}_j) = \begin{cases} f_{i+1/2,j}^I + \sigma_{i,j} \cdot \mathbf{x}, & \mathbf{x} \in \Omega_i, \\ f_{i+1/2,j}^O + \sigma_{i+1,j} \cdot \mathbf{x}, & \mathbf{x} \in \Omega_{i+1}, \end{cases} \quad (17)$$

where $\{f_{i+1/2,j}^I, f_{i+1/2,j}^O\}$ are the distribution functions at the face $\mathbf{x}_{i+1/2}$ reconstructed inside and outside the cell Ω_i , and $\{\sigma_i, \sigma_{i+1}\}$ are the spatial slopes that can be obtained with the help of various limiters. Note that under external force, in Eq. (16), $\mathbf{v}_k^0$ may not coincide with any node of the pre-established Eulerian mesh. The present study adopts central difference schemes to interpolate the value of the distribution function at this point.

A first-order Taylor expansion with respect to space and time is used to approximate the equilibrium distribution, i.e.,

$$\mathcal{M}(t, \mathbf{x}, \mathbf{v}) \approx \begin{cases} \mathcal{M}_0(1 + \theta_i \cdot \mathbf{x} + \phi t), & \mathbf{x} \in \Omega_i, \\ \mathcal{M}_0(1 + \theta_{i+1} \cdot \mathbf{x} + \phi t), & \mathbf{x} \in \Omega_{i+1}, \end{cases} \quad (18)$$

where $\mathcal{M}_0$ is the initial Maxwellian distribution function at $\{t = 0, \mathbf{x} = 0\}$, which can be determined using the compatibility condition of the kinetic equation, i.e.,

$$\begin{aligned} \int_{\mathbb{R}^3} \mathcal{M}_0 \psi d\mathbf{v} &= \int_{\mathbf{v} \cdot \mathbf{n} \geq 0} f_{i+1/2}^I \psi d\mathbf{v} + \int_{\mathbf{v} \cdot \mathbf{n} < 0} f_{i+1/2}^O \psi d\mathbf{v} \\ &\simeq \sum_{\mathbf{v}_j \cdot \mathbf{n} \geq 0} w_j f_{i+1/2,j}^I \psi_j + \sum_{\mathbf{v}_j \cdot \mathbf{n} < 0} w_j f_{i+1/2,j}^O \psi_j. \end{aligned} \quad (19)$$

The coefficients θ and ϕ represent the spatial and temporal slopes of the equilibrium distribution function, respectively. Since conservative variables are connected with the equilibrium distribution through moments over velocity space, the spatial and temporal derivatives of $\mathbf{W}$ can be expressed in terms of θ and ϕ as

$$\nabla_{\mathbf{x}} \mathbf{W} = \int_{\mathbb{R}^3} \theta \mathcal{M}_0 \psi d\mathbf{v}, \quad \frac{\partial \mathbf{W}}{\partial t} = \int_{\mathbb{R}^3} \phi \mathcal{M}_0 \psi d\mathbf{v}. \quad (20)$$

If we expand the slopes as linear combinations of ψ ,

$$\theta = \hat{\theta} \cdot \psi, \quad \phi = \hat{\phi} \cdot \psi, \quad (21)$$

where $\hat{\theta}$ and $\hat{\phi}$ are the combination coefficients of collision invariants, respectively. Eq. (20) can then be expressed as

$$\nabla_{\mathbf{x}} \mathbf{W} = \left(\int \mathcal{M}(\mathbf{v}) \psi(\mathbf{v}) \psi(\mathbf{v})^T d\mathbf{v} \right) \hat{\theta}, \quad (22a)$$

$$\frac{\partial \mathbf{W}}{\partial t} = \left(\int \mathcal{M}(\mathbf{v}) \psi(\mathbf{v}) \psi(\mathbf{v})^T d\mathbf{v} \right) \hat{\phi}. \quad (22b)$$

Eq. (22a) forms a linear system for $\hat{\theta}$ and can be solved formally as

$$\hat{\theta}(\mathbf{v}) = \left(\int \mathcal{M}(\mathbf{v}) \psi(\mathbf{v}) \psi(\mathbf{v})^T d\mathbf{v} \right)^{-1} \nabla_{\mathbf{x}} \mathbf{W}, \quad (23)$$

where the gradients $\nabla_{\mathbf{x}} \mathbf{W}$ can be approximated using central differences.

The temporal slopes can be approximated with the help of the Euler equations, i.e.,

$$\begin{aligned} \frac{\partial \mathbf{W}}{\partial t} &= - \int_{\mathbb{R}^3} \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathcal{M} \psi d\mathbf{v} - \int_{\mathbb{R}^3} \mathbf{a} \cdot \nabla_{\mathbf{v}} \mathcal{M} \psi d\mathbf{v} \\ &\approx - \int_{\mathbb{R}^3} \mathbf{v} \cdot \theta \mathcal{M}_0 \psi d\mathbf{v} - \int_{\mathbb{R}^3} \mathbf{a} \cdot \nabla_{\mathbf{v}} \mathcal{M} \psi d\mathbf{v}, \end{aligned} \quad (24)$$

where the gradients in velocity space $\nabla_{\mathbf{v}} \mathcal{M}$ can be solved theoretically. The temporal coefficients can be obtained analogously via

$$\hat{\phi} = \left(\int \mathcal{M}(\mathbf{v}) \psi(\mathbf{v}) \psi(\mathbf{v})^T d\mathbf{v} \right)^{-1} \frac{\partial \mathbf{W}}{\partial t}. \quad (25)$$

After all physical quantities and coefficients are determined, the integral solution in Eq. (16) becomes

$$\begin{aligned} f(t, 0, \mathbf{v}_j) &= (1 - e^{-t/\tau}) \mathcal{M}_{0,j} + (\tau(-1 + e^{-t/\tau}) + t e^{-t/\tau}) \theta_{i,i+1} \cdot \mathbf{v}_j \mathcal{M}_{0,j} \\ &\quad - \left[\tau(-1 + e^{-t/\tau}) + t e^{-t/\tau} + \frac{1}{2} t^2 e^{-t/\tau} \right] \theta_{i,i+1} \\ &\quad \cdot \mathbf{a} \mathcal{M}_{0,j} + \tau(t/\tau - 1 + e^{-t/\tau}) \phi \mathcal{M}_{0,j} \\ &\quad + e^{-t/\tau} \left[\left(f_{i+1/2,j}^I - \left(\mathbf{v}_j t - \frac{1}{2} \mathbf{a} t^2 \right) \cdot \sigma_{i,j} \right) H\left(-\mathbf{v}_j t + \frac{1}{2} \mathbf{a} t^2\right) \right. \\ &\quad \left. + \left(f_{i+1/2,j}^O - \left(\mathbf{v}_j t - \frac{1}{2} \mathbf{a} t^2 \right) \cdot \sigma_{i+1,j} \right) \left(1 - H\left(-\mathbf{v}_j t + \frac{1}{2} \mathbf{a} t^2\right) \right) \right] \\ &= \tilde{m}_j + \tilde{f}_j, \end{aligned} \quad (26)$$

which can be decomposed into the contributions from equilibrium and initial distribution functions. The generalized Heaviside function is defined as

$$H(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \Omega_i, \\ 0, & \mathbf{x} \in \Omega_{i+1}. \end{cases} \quad (27)$$

Finally, the numerical fluxes are determined by the time-dependent distribution function at the face, i.e.,

$$\begin{aligned} \mathbf{F}^f &= \mathbf{v} f(t, 0, \mathbf{v}), \\ \mathbf{F}^W &= \int_{\mathbb{R}^3} \mathbf{v} f(t, 0, \mathbf{v}) \psi d\mathbf{v}. \end{aligned} \quad (28)$$

3.3. Hermite approximation

For non-equilibrium flows under external force, a core task is to compute the derivatives of the distribution function in the velocity space. This study employs the Hermite polynomial expansion method proposed by Grad [32]. The distribution function is expanded as an N_m th order Hermite polynomial series, i.e.,

$$f(t, \mathbf{x}, \mathbf{v}) \approx f_{N_m} = \omega(\mathbf{u}) \sum_{n=0}^{N_m} \frac{1}{n!} \mathbf{d}^{(n)}(t, \mathbf{x}) : \mathcal{H}^{(n)}(\mathbf{u}), \quad (29)$$

where $\mathbf{u} = (\mathbf{v} - \mathbf{V})/\sqrt{RT}$ is the rescaled particle velocity based on local bulk velocity and temperature, R is the gas constant, $\omega(\mathbf{u}) \equiv \frac{1}{\sqrt{2\pi}^D} \exp(-\frac{\mathbf{u}^2}{2})$ is the weight function and D is the dimension. The tensor contraction is denoted as $:$. The n th order tensor Hermite polynomial is defined by

$$\mathcal{H}^{(n)}(\mathbf{u}) = \frac{(-1)^n}{\omega(\mathbf{u})} \nabla_{\mathbf{u}}^{(n)} \omega(\mathbf{u}), \quad (30)$$

which satisfies the recurrence relation, i.e.,

$$\mathcal{H}^{(n+1)}(\mathbf{u}) = \mathbf{u} \mathcal{H}^{(n)}(\mathbf{u}) - n \delta \mathcal{H}^{(n-1)}(\mathbf{u}), \quad (31)$$

with $\mathcal{H}^{(0)} = 1$, $\mathcal{H}^{(1)} = \mathbf{u}$, and δ the identity tensor. The expansion coefficients can be determined by

$$\begin{aligned} \mathbf{d}^{(n)}(t, \mathbf{x}) &= \int_{\mathbb{R}^D} f(t, \mathbf{x}, \mathbf{v}(\mathbf{u})) \mathcal{H}^{(n)}(\mathbf{u}) d\mathbf{u} \\ &= \frac{1}{(RT)^{D/2}} \int_{\mathbb{R}^D} f(t, \mathbf{x}, \mathbf{v}) \mathcal{H}^{(n)}(\mathbf{u}(\mathbf{v})) d\mathbf{v} \\ &\approx \frac{1}{(RT)^{D/2}} \sum_{j=1}^{N_v} w_j^{(\mathbf{v})} f_j \mathcal{H}_j^{(n)}. \end{aligned} \quad (32)$$

Notably, truncating the expansion in Eq. (29) at the zeroth-order ($N_m = 0$) recovers the Maxwellian distribution.

Substituting f_{N_m} into the forcing term of the Boltzmann equation yields

$$\begin{aligned} \mathbf{a} \cdot \nabla_{\mathbf{v}} f &\approx \frac{1}{\sqrt{RT}} \mathbf{a} \cdot \nabla_{\mathbf{u}} \left(\omega(\mathbf{u}) \sum_{n=0}^{N_m} \frac{1}{n!} \mathbf{d}^{(n)}(t, \mathbf{x}) : \mathcal{H}^{(n)}(\mathbf{u}) \right) \\ &= \frac{1}{\sqrt{RT}} \mathbf{a} \cdot \sum_{n=0}^{N_m} \frac{1}{n!} \mathbf{d}^{(n)}(t, \mathbf{x}) : \mathbf{f}_{\mathbf{u}}(\omega(\mathbf{u}) \mathcal{H}^{(n)}(\mathbf{u})) \\ &= -\frac{1}{\sqrt{RT}} \omega(\mathbf{u}) \sum_{n=0}^{N_m} \frac{1}{n!} \mathbf{a} \otimes \mathbf{d}^{(n)}(t, \mathbf{x}) : \mathcal{H}^{(n+1)}(\mathbf{u}). \end{aligned} \quad (33)$$

By substituting the Hermite polynomials and moments, the above equation can be further simplified as

$$\begin{aligned} \mathbf{a} \cdot \nabla_{\mathbf{v}} f &\approx -\frac{1}{\sqrt{RT}} \mathcal{M} \left(\mathbf{a} \cdot \mathbf{u} + \frac{\mathbf{a} \otimes \mathbf{T}}{2\rho RT} : \mathcal{H}^{(3)}(\mathbf{u}) \right. \\ &\quad \left. + \frac{\mathbf{a} \otimes \mathbf{Q}}{6\rho(RT)^{3/2}} : \mathcal{H}^{(4)}(\mathbf{u}) + \dots \right), \end{aligned} \quad (34)$$

where the modified stress and heat transfer tensors are defined as

$$\mathbf{T} = \int_{\mathbb{R}^3} RT f(\mathbf{u} \otimes \mathbf{u} - \delta) d\mathbf{v}, \quad \mathbf{Q} = \int_{\mathbb{R}^3} (RT)^{3/2} f(\mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u}) d\mathbf{v}. \quad (35)$$

It can be seen that the leading term in Eq. (34) describes the equilibrium effects of external force, while the rest higher-order terms quantify the non-equilibrium effects. The Hermite expansion conserves the moments of external force up to $(N_m + 1)$ th order.

The spectral convergence of Hermite expansions undoubtedly provides an efficient tool to characterize the non-equilibrium distribution function and compute its derivatives. The other remaining question to address is its universality. As analyzed in [32], provided that $\omega^{-1/2} f$ is square integrable, the series in Eq. (29) converges spectrally. The necessary condition is

$$\lim_{|\mathbf{v}| \rightarrow \infty} f \exp \left(\frac{|\mathbf{v} - \mathbf{V}|^2}{4RT} \right) = 0. \quad (36)$$

This implies that the velocity distribution to be approximated must decay at a faster rate than the exponential factor $\exp(-|\mathbf{v} - \mathbf{V}|^2/4RT)$, which can be regarded as an equilibrium distribution with the temperature $2T$. For most non-equilibrium distributions, this condition can be naturally satisfied. Occasionally, in highly dissipative regions, e.g., in the vicinity of a shock wave with a large temperature gradient, the scaled temperature may be chosen (to surpass no less than half of the domain's peak temperature) as a surrogate of the local temperature T to guarantee the convergence of the series [33,34]. The detailed numerical implementation of the Hermite spectral method can be found in Appendix A.

3.4. Numerical quadrature

The numerical integration based on a particle distribution function can be written as

$$\int_{\mathbb{R}^3} g(\mathbf{v}) f(\mathbf{v}) d\mathbf{v} \approx \sum_j^{N_v} w_j g(\mathbf{v}_j) f(\mathbf{v}_j), \quad (37)$$

where g denotes an arbitrary function of $\mathbf{v}$, and w_j is the quadrature weight at the collocation point $\mathbf{v}_j$. Two sets of numerical quadratures are considered in this study to solve the BGK equation. For brevity, we describe their use in the one-dimensional case below, while the extension to the multi-dimensional case is straightforward via the tensor product rule.

The first numerical quadrature follows the Newton-Cotes (NC) rule. This method samples the integrand at equally spaced points. The quadrature weights are determined by integrating the Lagrange basis polynomials over the velocity space. If the integrand is sufficiently smooth, it

can be proved that the error scaling of the Newton-Cotes rule follows

$$|\epsilon| \leq C(\Delta v)^p \max_{v \in [-V, V]} |I^{(p)}(v)|, \quad (38)$$

Here I denotes the integrand, while p and C depend on the selected composite Newton-Cotes rule.

The second numerical quadrature is the Gauss-Hermite (GH) quadrature. This technique is tailored to approximate integrals of the form

$$\int_{-\infty}^{\infty} e^{-v^2} I(v) dv \approx \sum_{j=1}^{N_v} w_j I(v_j). \quad (39)$$

The quadrature nodes are placed at the N_v real roots of N_v th Hermite polynomial (as discussed in Section 3.3), and the weights are given by

$$w_j = \frac{2^{N_v-1} N_v! \sqrt{\pi}}{N_v^2 [H_{N_v-1}^{\text{phys}}(v_j)]^2}, \quad H_{N_v}^{\text{phys}}(v_j) = 0. \quad (40)$$

The Gauss-Hermite quadrature is especially efficient for those quadrature problems in which the integrand is multiplied by e^{-v^2} , e.g., the Maxwellian distribution function. It can be applied to an arbitrary integrand by refactoring it to match the Hermite-weight form, i.e.,

$$I^*(v) = e^{v^2} I(v), \quad \int_{-\infty}^{\infty} I(v) dv = \int_{-\infty}^{\infty} e^{-v^2} I^*(v) dv \approx \sum_{j=1}^{N_v} w_j I^*(v_j). \quad (41)$$

The quadrature is exact when the integrand is a polynomial of degree up to $2N_v - 1$. Note that besides the classic Gauss-Hermite quadrature, the quadrature nodes can also be shifted and rescaled to adapt peculiar non-equilibrium distributions.

3.5. Well-balanced property

The well-balanced property is achieved due to the precise offset of the external forcing terms and inhomogeneous fluxes in Eq. (9) (and Eq. (10), correspondingly). Here, we analyze the numerical behavior of the solution algorithm in the asymptotic limit of the BGK equation. For brevity, a local coordinate system aligned with the direction of the external force is established, thereby simplifying the flow equations to one dimension. In the continuum limit, i.e., the Euler equations, the hydrostatic equilibrium solution takes the form

$$\rho = \rho_0 \exp \left(\frac{ax}{RT} \right), \quad \mathbf{V} = 0, \quad p = p_0 \exp \left(\frac{ax}{RT} \right), \quad (42)$$

where $\{\rho_0, p_0\}$ are the density and pressure at an arbitrarily selected reference state. The temperature T is equal everywhere [3]. With infinitely frequent intermolecular collisions, the particle distribution function is everywhere in equilibrium.

We first consider the source term part. Provided that the particle distribution function is Maxwellian, the Hermite expansion in Eq. (34) degenerates to

$$G = -\mathbf{a} \cdot \nabla_{\mathbf{v}} f = -\frac{a\mathbf{u}}{RT} \mathcal{M}, \quad (43)$$

and the source terms related to the external force can be obtained via

$$\mathbf{G} = \int G \psi d\mathbf{v} = \begin{pmatrix} 0 \\ \rho a \\ \rho U a \end{pmatrix} = \begin{pmatrix} 0 \\ \rho a \\ 0 \end{pmatrix}. \quad (44)$$

Since the zeroth-order truncation in the Hermite expansion corresponds to the Maxwellian distribution, the two source terms above do not introduce any numerical errors.

We then turn to the numerical fluxes. In the Euler limit with $\tau \rightarrow 0$, the integral solution in Eq. (26) reduces to

$$f = \mathcal{M}_0(1 + \mathbf{t}\phi). \quad (45)$$

As analyzed in Section 3.2, the temporal slope of the distribution function can be obtained via

$$-\int u \partial_x \mathcal{M} \psi du - \int a \partial_v \mathcal{M} \psi du = \frac{\partial W}{\partial t} = \int \phi \mathcal{M} \psi du. \quad (46)$$

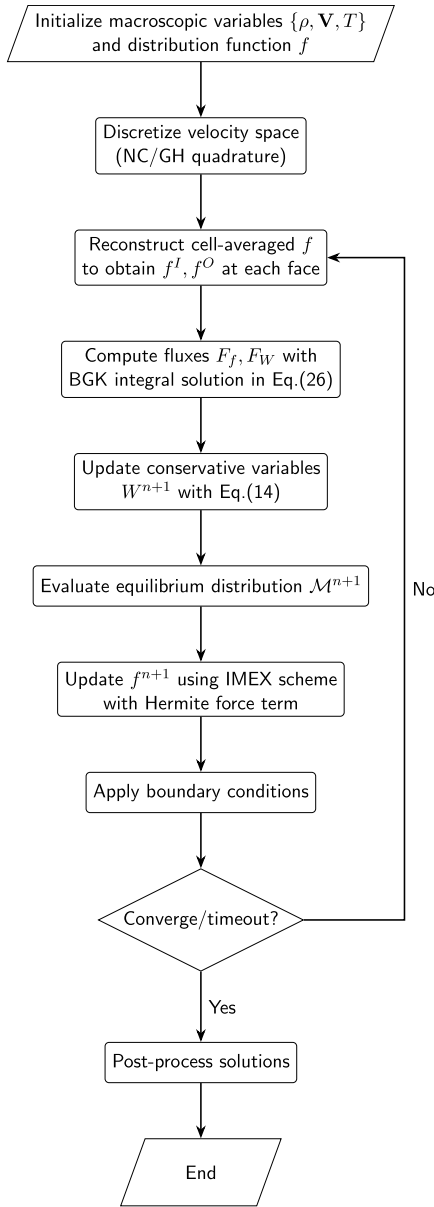


Fig. 1. Workflow of the proposed solution algorithm.

The derivatives of the Maxwellian distribution can be obtained using the chain rule, i.e.,

$$\begin{aligned}\frac{\partial \mathcal{M}}{\partial x} &= \frac{1}{\rho} \frac{\partial \rho}{\partial x} \mathcal{M} + \frac{1}{2\lambda} \frac{\partial \lambda}{\partial x} \mathcal{M} - (u^2 - 2uU + U^2) \frac{\partial \lambda}{\partial x} \mathcal{M} + 2\lambda(u - U) \frac{\partial U}{\partial x} \mathcal{M}, \\ \frac{\partial \mathcal{M}}{\partial u} &= -2\lambda(u - U) \mathcal{M},\end{aligned}\quad (47)$$

where $\lambda = 1/(2RT)$. Inserting the hydrostatic solution in Eq. (42) yields $\phi = 0$.

Therefore, the numerical fluxes depend only on the Maxwellian distribution at the cell face, which are of the form

$$\begin{aligned}\mathbf{F}^f &= u\mathcal{M}_0, \\ \mathbf{F}^W &= \int_{-\infty}^{\infty} u\mathcal{M}_0 \psi du = \begin{pmatrix} 0 \\ \rho RT \\ 0 \end{pmatrix}.\end{aligned}\quad (49)$$

It is clear that density and energy are well balanced. For the momentum equation, we can obtain the following relation between the source term and numerical flux, i.e.,

$$\begin{aligned}\int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{G}_i^{\rho U} dx &= \int_{x_{i-1/2}}^{x_{i+1/2}} \rho adx \\ &= RT(\rho_{x_{i+1/2}} - \rho_{x_{i-1/2}}) = -(\mathbf{F}_{i-1/2}^{\rho U} - \mathbf{F}_{i+1/2}^{\rho U}).\end{aligned}\quad (50)$$

from which the well balance in a control volume is clearly identified.

The above analysis is performed only in the asymptotic limit with vanishing molecular mean free path. When the mean free path is not zero (i.e., the flow regimes of Navier-Stokes equations and beyond), it can be shown that there exist non-equilibrium stress and heat flux aligned with the direction of the external force, and thus the hydrostatic solution is no longer isothermal [7]. It is difficult to prove the well-balanced property by numerical analysis anymore. It should be noted, however, that it is the non-equilibrium effects described above where the role of external forces becomes exceptionally important. By introducing particle trajectories under external forces into the numerical flux function (from the integral solution of the BGK equation) and solving exactly for the derivatives in the phase space (using the Hermite spectral method), the current solution algorithm is consistent with the physical mechanisms of multi-scale flow transport, and should consequently demonstrate superior performance in non-equilibrium flow simulations. In the next section, we will conduct numerical experiments to validate the efficacy of the solution algorithm.

Algorithm 1 Algorithm flowchart of the solution method.

- 1: **Input:** prescribed flow configuration; computational mesh; velocity quadrature.
- 2: **Initialization**
Set initial macroscopic variables $(\rho, \mathbf{V}, T)$ and distribution function f ;
Discretize the velocity space using Newton–Cotes or Gauss–Hermite quadrature.
- 3: **while** not satisfying the convergence criterion **do**
- 4: **Flux computation**
Reconstruct interface values f^I and f^O using a slope limiter;
Compute conservative variables at the face $\mathbf{W}_0 = \int f \psi d\mathbf{v}$ and evaluate $\mathcal{M}_0$ in Eq. (18);
Compute spatial slope θ and temporal slope ϕ according to Eqs. (20) to (25);
Compute the BGK integral solution in Eq. (26) to obtain the numerical fluxes F_f and F_W .
- 5: **Update of macroscopic variables**
Update conservative variables using Eq. (14);
Evaluate the equilibrium distribution $\mathcal{M}^{n+1}$ using Eq. (3).
- 6: **Update of distribution function**
Compute the external forcing term using the Hermite spectral method in Eq. (34);
Update f using the IMEX scheme in Eq. (13).
- 7: **Boundary treatment and time control**
Apply specific boundary conditions;
Determine the time step Δt based on the CFL condition in physical and velocity space.
- 8: **end while**
- 9: **Post-processing**
Compute necessary macroscopic variables by taking moments of f ;
Export field solution and visualize;
Analyze field solution systematically.
- 10: **Output:** Solution datasets, visualizations, and analysis results.

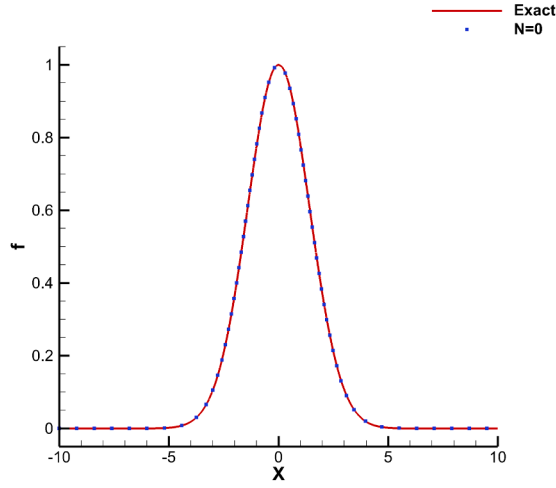
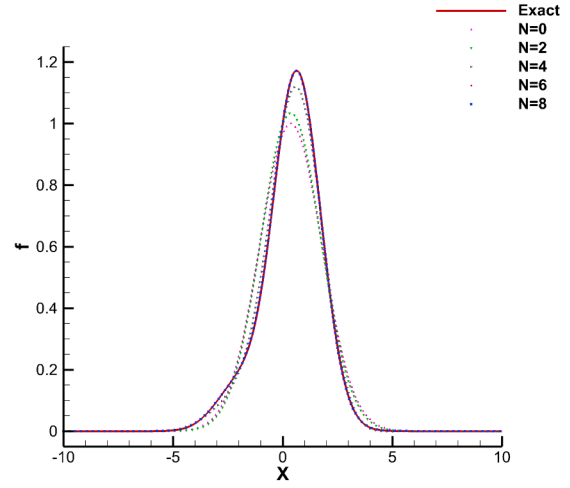
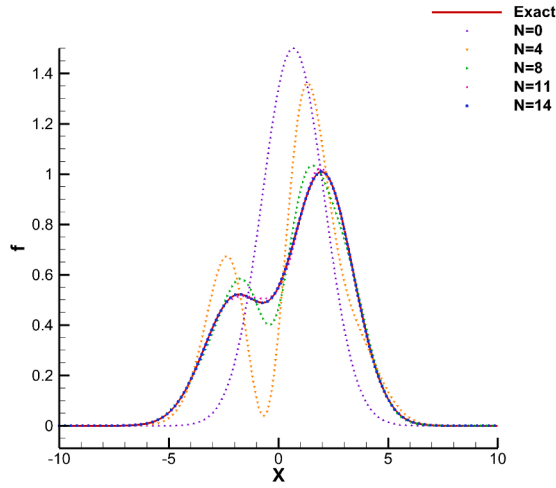
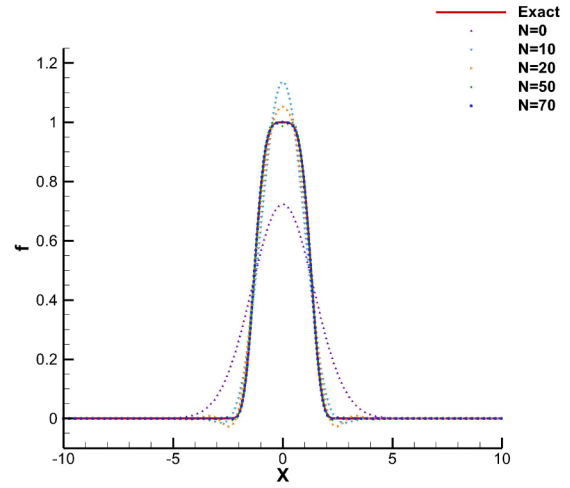
(a) $f = \exp(-\frac{1}{4}u^2)$ (b) $f = \exp(-\frac{1}{4}u^2)(1 + 0.5 \sin(u))$ (c) $f = \exp(-\frac{1}{4}(u-2)^2) + \frac{1}{2} \exp(-\frac{1}{4}(u+2)^2)$ (d) $f = \exp(-\frac{1}{4}u^4)$

Fig. 2. Convergence tests of the Hermite approximation of near-equilibrium and non-equilibrium particle distribution functions. Here, N represents the order of the Hermite expansion.

3.6. Numerical implementation

To ensure reproducibility, the proposed solution algorithm has been implemented within a modular computational framework. Its workflow follows the algorithm flow chart illustrated in Fig. 1 and is summarized in Algorithm 1. The implementation strictly adheres to the theoretical formulations presented in Sections 3.1–3.5. The key components are summarized below.

- (i) **Initialization.** The computational domain is divided into control volumes, and the velocity space is discretized within a suitable quadrature (e.g., the Newton–Cotes or Gauss–Hermite). Macroscopic variables $\{\rho, \mathbf{V}, T\}$ are initialized according to the specified flow conditions, and the initial distribution function f is set to its Maxwellian equilibrium $\mathcal{M}$.
- (ii) **Flux computation.** At each time step, the distribution function $f_{i,j}$ is reconstructed within each cell to approximate the inner and outer values $\{f_{i+1/2,j}^I, f_{i+1/2,j}^O\}$ at the face $\mathbf{x}_{i+1/2}$. The macroscopic variables at the face are then determined from the velocity moments of these reconstructed distributions, and the local equilib-

rium distribution $\mathcal{M}_0$ is evaluated accordingly. The spatial gradients of the macroscopic variables are computed by central differences to determine the spatial slope θ , while the temporal slope ϕ is obtained with the help of the Euler equations, according to Eqs. (20) to (25). Having obtained all necessary components, the integral solution of the BGK equation in Eq. (26) is utilized to yield the time-dependent distribution function. The numerical fluxes F_f and F_w are then computed from this distribution and used to update the macroscopic and microscopic variables for the next time step.

- (iii) **Update of macroscopic variables.** The conservative variables are updated using Eq. (14), after which the corresponding equilibrium distribution function $\mathcal{M}^{n+1}$ is evaluated using Eq. (3).
- (iv) **Update of distribution function.** The implicit–explicit scheme (IMEX) in Eq. (13) is employed to update the distribution function. The external forcing term associated with velocity-space derivatives is computed using the Hermite spectral method, as illustrated in Eq. (34).
- (v) **Boundary and time control.** Boundary conditions are applied according to the specific problem settings. The time step Δt is

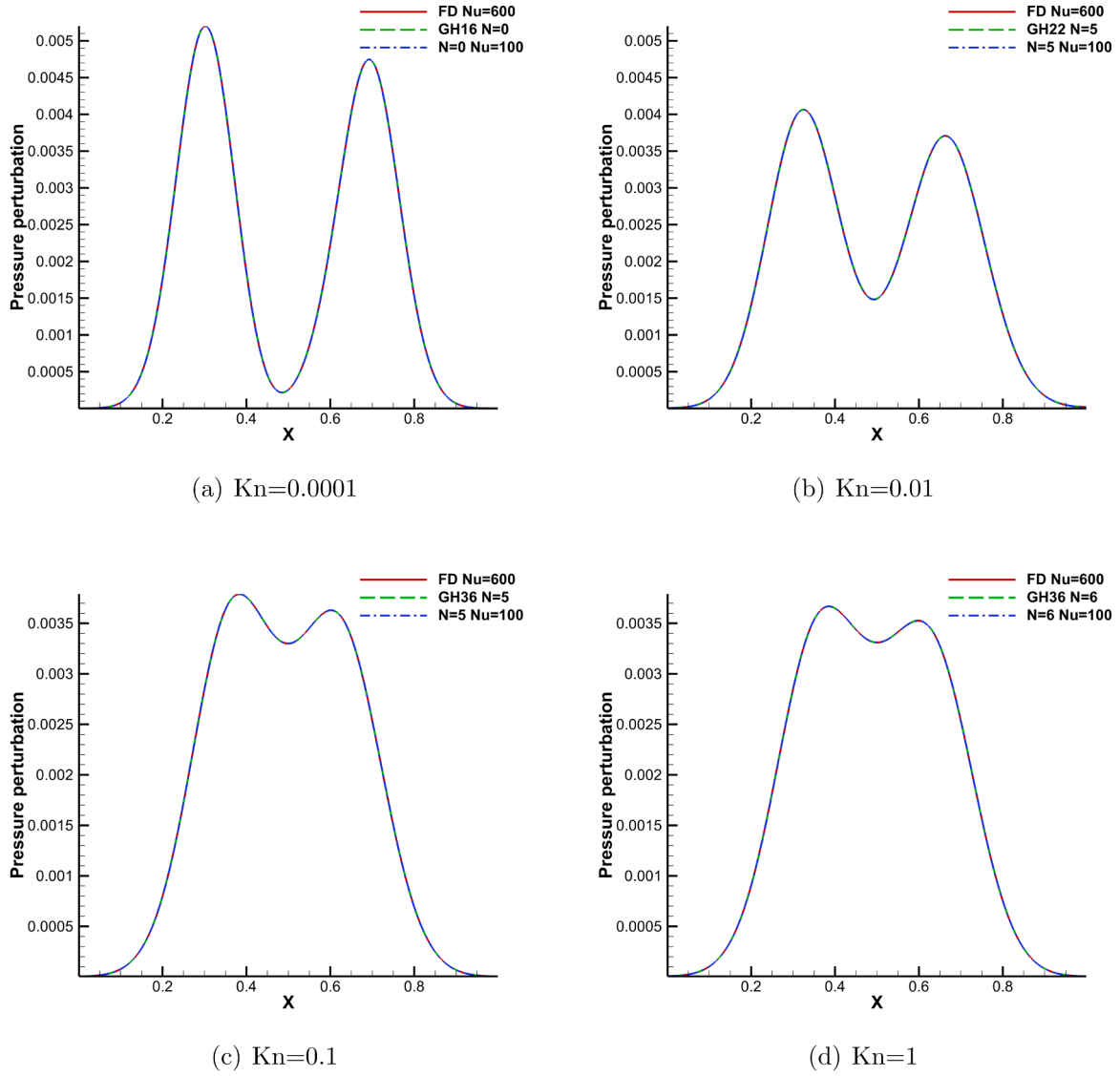


Fig. 3. Pressure perturbation distributions from hydrostatic solution at different reference Knudsen numbers. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

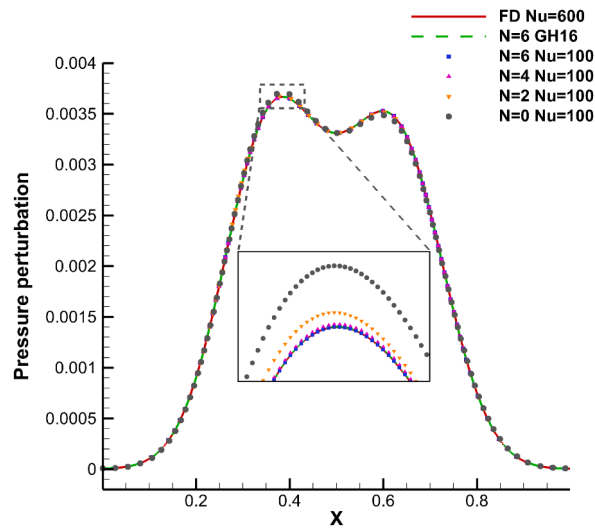


Fig. 4. Convergence test and criterion for determining the order of Hermite polynomials in one-dimensional hydrostatic problem (with $Kn = 1$).

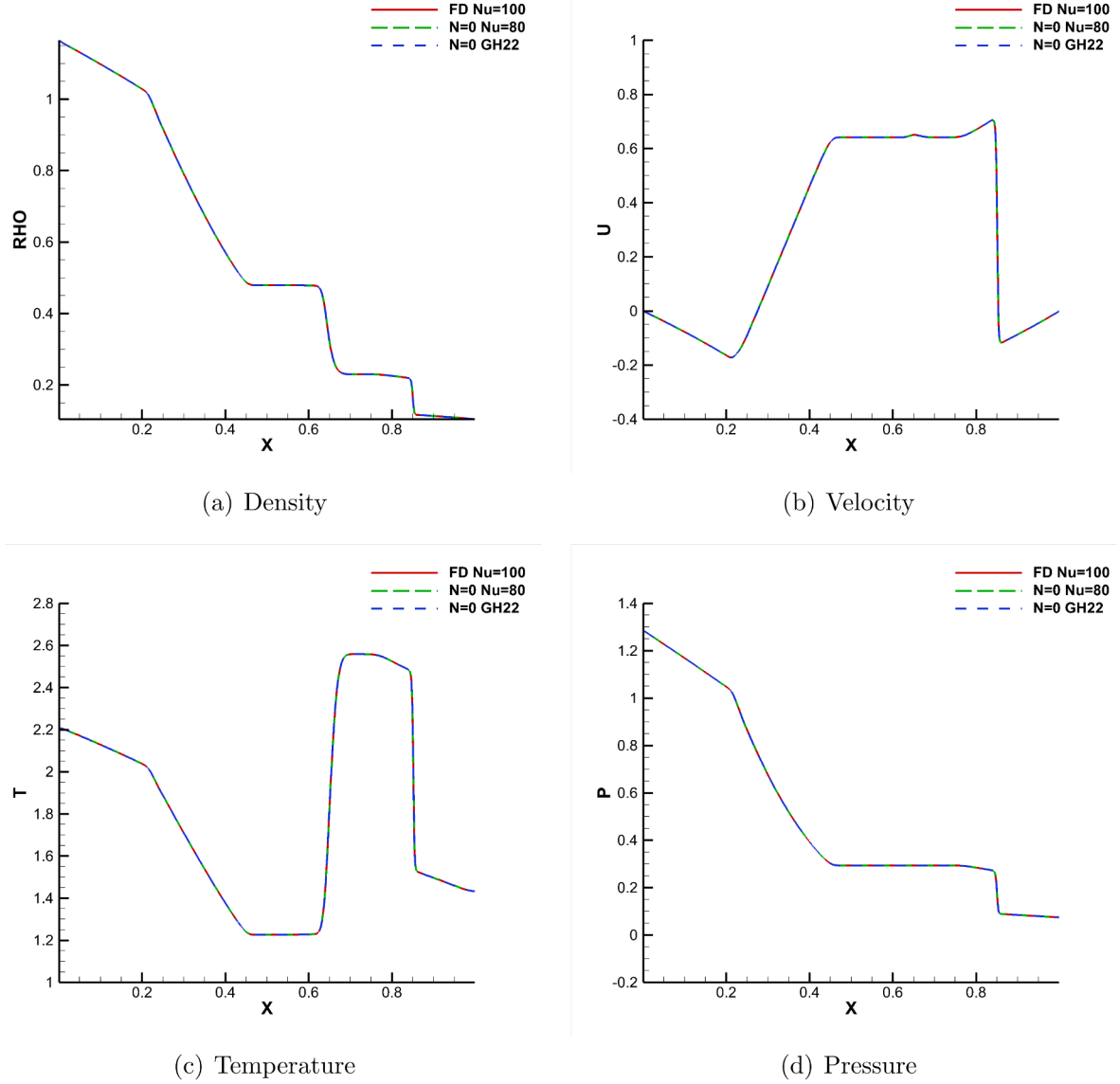


Fig. 5. Distributions of flow variables in the Sod shock tube under external force at $\text{Kn}=0.0001$. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

determined adaptively via the CFL condition based on the propagation of information in both physical and velocity space.

- (vi) **Post-processing.** Collect the updated macroscopic variables and distribution function. Necessary moments, e.g., the stress and heat flux, can be computed using the distribution function. The field solution is visualized and systematically analyzed.

A numerical implementation of the proposed solution algorithm has been developed in Fortran. The implementation utilizes vectorized operations to efficiently compute Hermite coefficients and scale-dependent numerical fluxes. Appendix A details the implementation specifics. Its modular structure enables seamless extension to three-dimensional configurations and hybrid CPU-GPU computational architectures. The simulation program has been validated through comprehensive numerical experiments in Section 4, demonstrating consistent accuracy and numerical stability across a broad range of Knudsen numbers and forcing magnitudes.

4. Numerical experiments

Numerical experiments are presented in this section to validate the current solution algorithm. Dimensionless variables are introduced as

$$\begin{aligned} \tilde{t} &= \frac{t}{L_0/V_0}, \quad \tilde{x} = \frac{x}{L_0}, \quad \tilde{\rho} = \frac{\rho}{\rho_0}, \quad \tilde{\mathbf{V}} = \frac{\mathbf{V}}{V_0}, \quad \tilde{T} = \frac{T}{T_0}, \quad \tilde{E} = \frac{E}{V_0^2}, \\ \tilde{\mathbf{P}} &= \frac{\mathbf{P}}{\rho_0 V_0^2}, \quad \tilde{\mathbf{q}} = \frac{\mathbf{q}}{\rho_0 V_0^3}, \quad \tilde{\mathbf{v}} = \frac{\mathbf{v}}{V_0}, \quad \tilde{f} = \frac{f}{\rho_0/V_0^3}, \quad a_0 = \frac{V_0^2}{L_0}, \quad \tilde{\mathbf{a}} = \frac{\mathbf{a}}{a_0} = \frac{L_0 \mathbf{a}}{V_0^2}, \end{aligned} \quad (51)$$

where a physical quantity with a subscript of 0 indicates its value in the reference state, $V_0 = \sqrt{2kT_0/m}$ is the most probable molecular speed. The referenced Knudsen number is defined as

$$\text{Kn} = \frac{\ell_0}{L_0} = \frac{V_0}{L_0 \nu_0}, \quad (52)$$

where $\ell_0 = V_0/\nu_0$ denotes the molecular mean free path and ν_0 is the mean collision frequency. Based on the variable hard sphere (VHS)

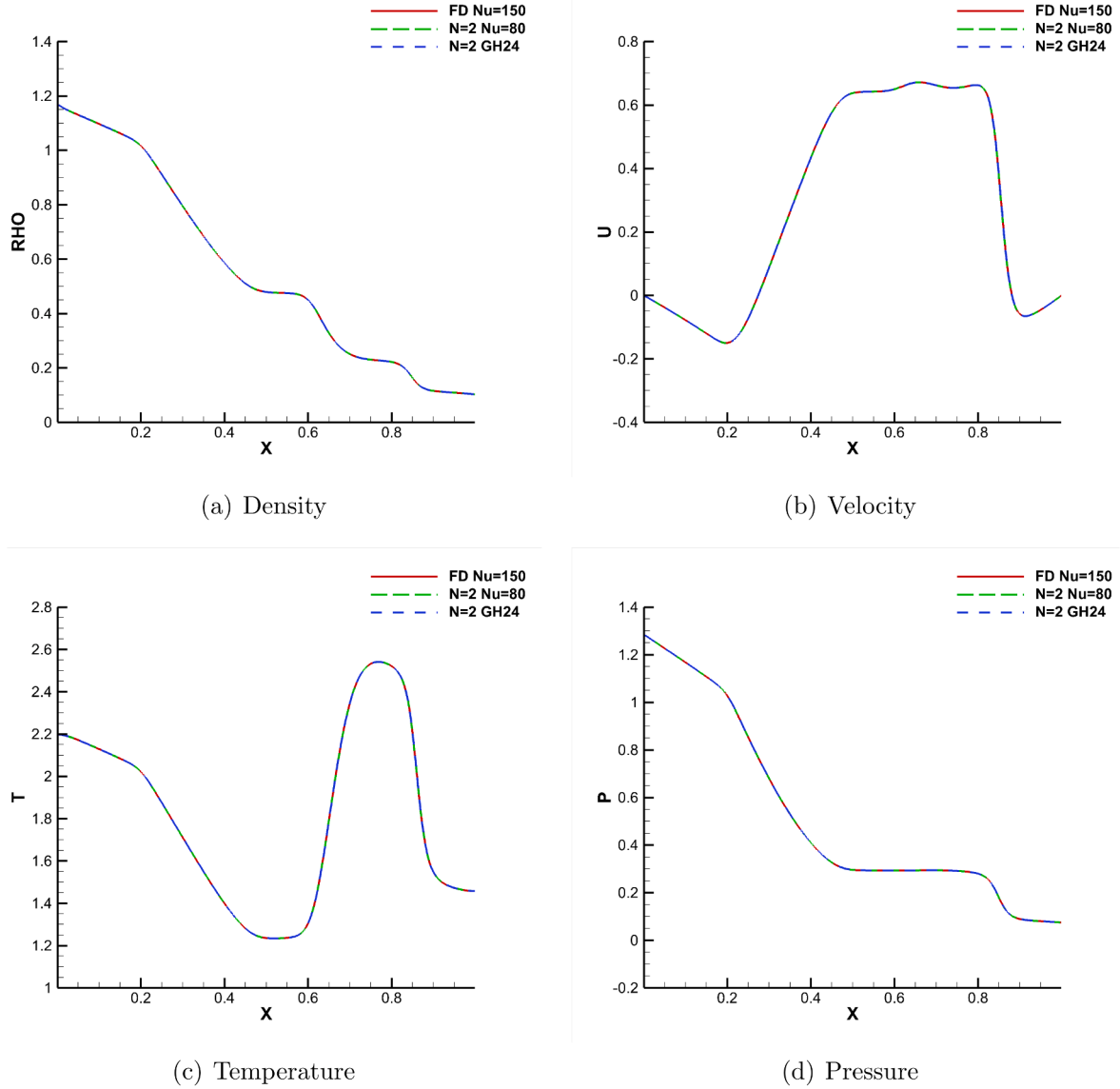


Fig. 6. Distributions of flow variables in the Sod shock tube under external force at $\text{Kn}=0.001$. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

model, the reference viscosity can be expressed in a dimensionless form as

$$\mu_{ref} = \frac{5(\alpha+1)(\alpha+2)\sqrt{\pi}}{4\alpha(5-2\eta)(7-2\eta)} \text{Kn}, \quad (53)$$

and the relaxation time τ is given by

$$\tau = \frac{2\mu_{ref}}{\rho} T^{\eta-1}. \quad (54)$$

where α is the scattering parameter (with $\alpha=1$ for the hard sphere model) and ω is the viscosity index (e.g., $\eta=0.81$ for argon). For brevity, we drop the tilde notation to denote dimensionless variables henceforth.

4.1. Convergence of hermite approximation

The first numerical experiment examines the convergence properties of the Hermite approximation when applied to particle distributions in both near-equilibrium and non-equilibrium states. Four forms of the particle distribution function are considered, i.e.,

$$1. f = \exp(-\frac{1}{4}u^2),$$

$$2. f = \exp(-\frac{1}{4}u^2)(1 + 0.5 \sin(u)),$$

$$3. f = \exp(-\frac{1}{4}(u-2)^2) + \frac{1}{2} \exp(-\frac{1}{4}(u+2)^2),$$

$$4. f = \exp(-\frac{1}{4}u^4).$$

Fig. 2 illustrates the approximation of four distribution functions using the Hermite expansion. It can be seen that the numerical accuracy and rate of convergence are strongly correlated with the form of the distribution function. For equilibrium and near-equilibrium distributions, since the first term of the Hermite expansion corresponds to the Maxwellian distribution, the distribution function can be accurately characterized with minimal expansion orders. For non-equilibrium distributions, the Hermite spectral method also exhibits good convergence properties. Merely $O(10)$ expansion terms are required to precisely resolve typical non-equilibrium distributions, e.g., the bimodal distribution shown in **Fig. 2(c)**. Compared to the finite difference discrete velocity method, this method offers substantially superior computational efficiency (which will be corroborated by our numerical experiments starting from **Section 4.2**). When the distribution function is sharply located or discontinuous in the velocity space, e.g., in **Fig. 2(d)**, Gibbs' phenomenon leads to the need for higher orders of expansion to converge

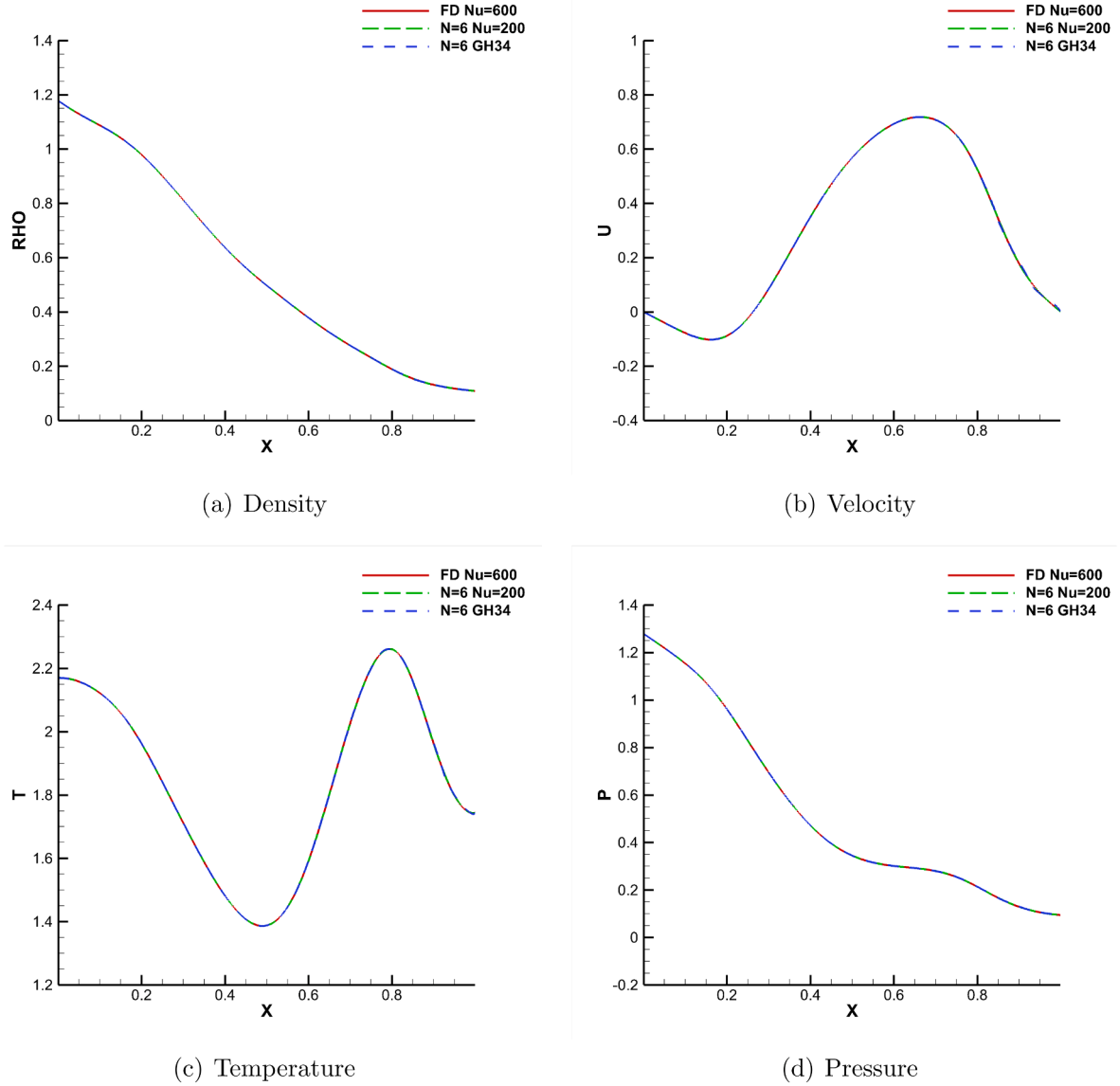


Fig. 7. Distributions of flow variables in the Sod shock tube under external force at $Kn = 0.01$. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

to the accurate distribution. Fortunately, such non-trivial distributions rarely occur in space and time in real-world flow problems. Throughout the computational cycle, the Hermite approximation is capable of providing efficient and accurate characterization of distribution functions in most cases.

4.2. One-dimensional hydrostatic solution

We then verify the well-balanced property of the solution algorithm. The one-dimensional, dimensionless hydrostatic solution is set as

$$\rho_0 = \exp(ax), \quad U_0 = 0, \quad p_0 = \exp(ax). \quad (55)$$

The pressure field is then subjected to the following perturbation,

$$p = p_0(x) + 0.01e^{-100(x-0.5)^2}. \quad (56)$$

The initial particle distribution function is set as Maxwellian everywhere in correspondence with the macroscopic variables. The detailed computational setup is provided in Table 2.

Fig. 3 presents the spatial distribution of pressure perturbations at the output moment. As discussed in [35], a naive treatment of the external force term can fail to capture such a small perturbation without

destroying the global hydrostatic solution. Thanks to the well-balanced property, the current solution algorithm accurately captures the propagation of pressure perturbations in different flow regimes. Table 3 lists the computational costs of different methods (i.e., the Hermite approximation in Section 3.3 and second-order central difference) in the same framework. The results show that the Hermite spectral method, along with the Gauss-Hermite quadrature, significantly improves the computational efficiency of the numerical method at different reference Knudsen numbers (more than one order of magnitude improvement over the finite difference method). The computational parameters in the table are determined by the grid convergence tests. Fig. 4 illustrates a typical convergence test case for determining the order of Hermite polynomials.

4.3. Shock tube under external force

We then test the capability of the solution algorithm for solving discontinuous solutions. The Sod shock tube is employed as the numerical experiment. The particle distribution function is initialized as Maxwellian in the whole flow domain, which corresponds to the

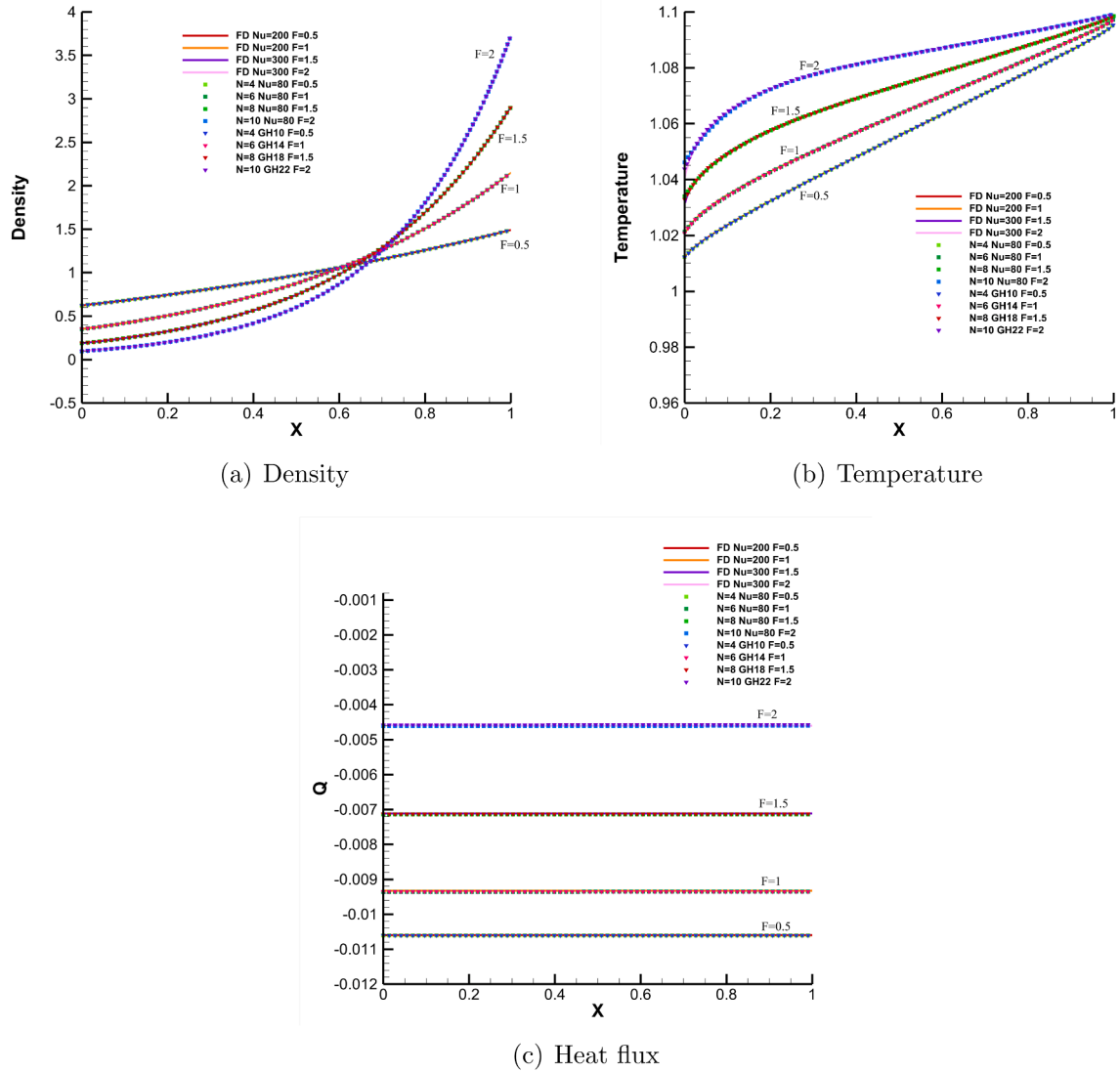


Fig. 8. Distributions of density, temperature, and heat flux in one-dimensional Fourier flow problem under different external forces at $\text{Kn} = 0.1$. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

Table 2

Computational setup of one-dimensional hydrostatic problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Gas	t	x	N_x	u	N_u	Order
Argon	(0, 0.1]	[0, 1]	600	$[-5, 5]$	[16, 600]	2
N_m	a	Kn	Quadrature	Integrator	Boundary	CFL
[0, 6]	-1	[0.0001, 1]	NC/GH	IMEX	Dirichlet	0.5

following macroscopic variables,

$$\begin{pmatrix} \rho \\ U \\ p \end{pmatrix}_{t=0, x<0.5} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} \rho \\ U \\ p \end{pmatrix}_{t=0, x \geq 0.5} = \begin{pmatrix} 0.125 \\ 0 \\ 0.1 \end{pmatrix}. \quad (57)$$

The detailed computational setup is described in Table 4.

Figs. 5–7 present the spatial distribution of macroscopic variables at the output moment under different Knudsen numbers. Under the external force field, particles in the region where the waves have not arrived are driven to the left. This numerical experiment demonstrates the well-balanced and asymptotic-preserving properties of the current scheme. The evolution of discontinuities is well captured under the force field in different flow regimes. With the increasing Knudsen number, a continu-

Table 3

Computational costs of different methods for solving the one-dimensional hydrostatic problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Knudsen number	Numerical method	Number of collocation points	Time (s)
0.0001	finite difference (NC)	600	85.19
	Hermite (NC, $N_m = 0$)	100	20.17
	Hermite (GH, $N_m = 0$)	16	2.48
0.01	finite difference (NC)	600	85.14
	Hermite (NC, $N_m = 5$)	100	37.96
	Hermite (GH, $N_m = 5$)	22	4.20
0.1	finite difference (NC)	600	81.02
	Hermite (NC, $N_m = 6$)	100	41.69
	Hermite (GH, $N_m = 6$)	36	4.47
1	finite difference (NC)	600	81.12
	Hermite (NC, $N_m = 6$)	100	53.49
	Hermite (GH, $N_m = 6$)	36	4.59

ous spectrum of flow physics is recovered from the Boltzmann solution to the Euler solution of the one-dimensional Riemann problem.

Table 5 lists the computational costs of different methods (i.e., the Hermite approximation in Section 3.3 and second-order central

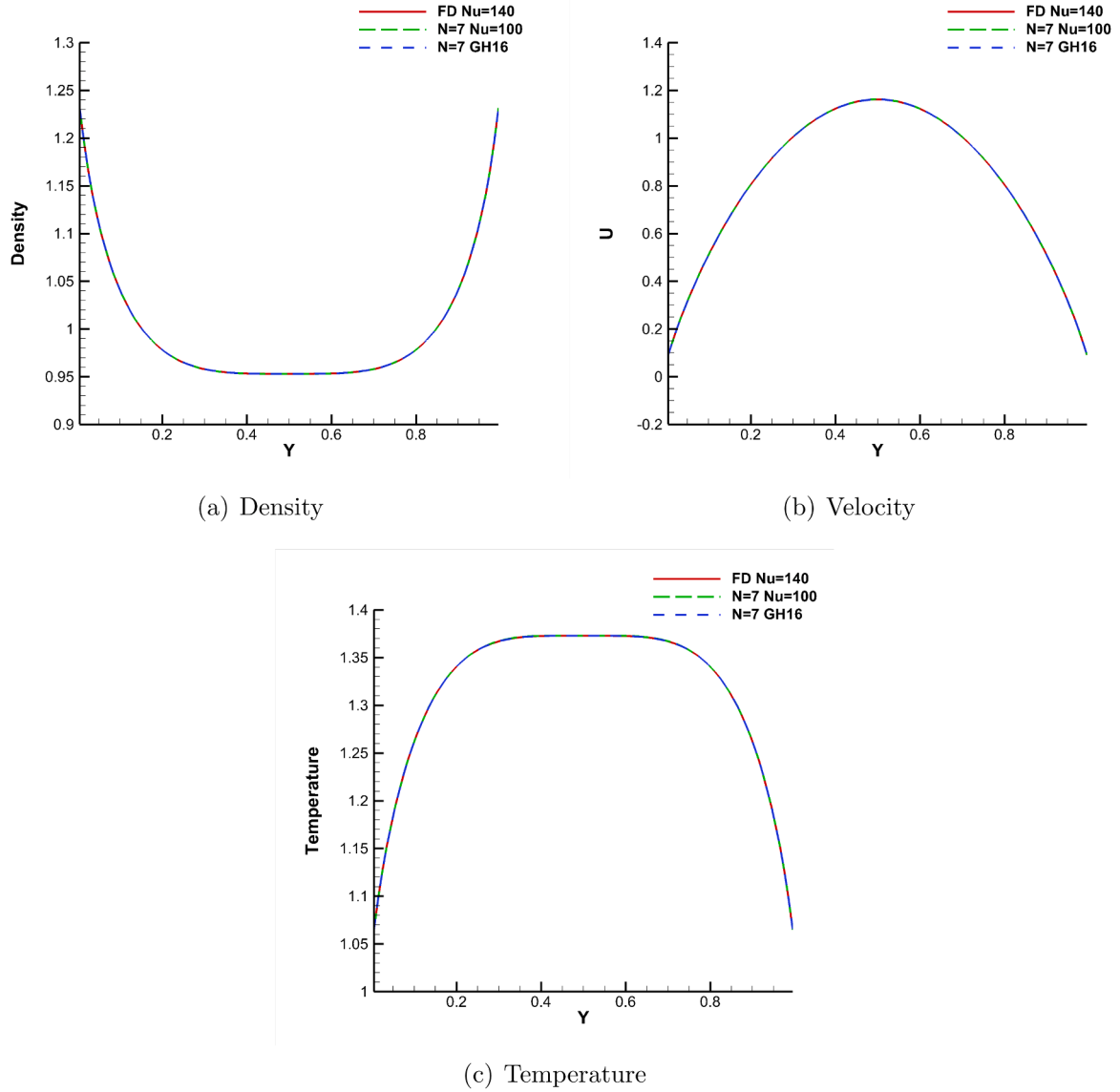


Fig. 9. Distributions of density, velocity, and temperature in the Poiseuille flow problem at $Kn=0.02$. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

Table 4

Computational setup of Sod shock tube problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Gas	t	x	N_x	u	N_u	Order
Argon	(0, 0.2]	[0, 1]	600	$[-5, 5]$	[22, 600]	2
N_m	a	Kn	Quadrature	Integrator	Boundary	CFL
[0, 6]	-1	[0.0001, 0.01]	NC/GH	IMEX	Dirichlet	0.5

difference) for the numerical solution in the same framework. The results show that the Hermite spectral method, along with the Gauss-Hermite quadrature, significantly improves the computational efficiency of the numerical method at different reference Knudsen numbers. The amount of computational degrees of freedom and overall time have been reduced by 80%.

4.4. Fourier flow

Subsequently, we examine the capability of the solution algorithm for solving energy transport. The Fourier flow between two infinitely

Table 5

Computational costs of different methods for solving the Sod shock tube problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Knudsen number	Numerical method	Number of collocation points	Time (s)
0.0001	finite difference (NC)	100	59.06
	Hermite (NC, $N_m = 0$)	80	41.19
	Hermite (GH, $N_m = 0$)	22	9.29
0.001	finite difference (NC)	150	106.25
	Hermite (NC, $N_m = 2$)	80	68.82
	Hermite (GH, $N_m = 2$)	24	15.80
0.01	finite difference (NC)	600	227.54
	Hermite (NC, $N_m = 6$)	200	220.77
	Hermite (GH, $N_m = 6$)	34	44.82

large parallel plates is employed as the numerical experiment, where the temperatures of the upper and lower plates are set as 1.1 and 1.0, respectively. The initial flow field is set up with a fixed temperature, and the particle distribution function is initialized as Maxwellian in the whole computational domain. The effect of external force fields of

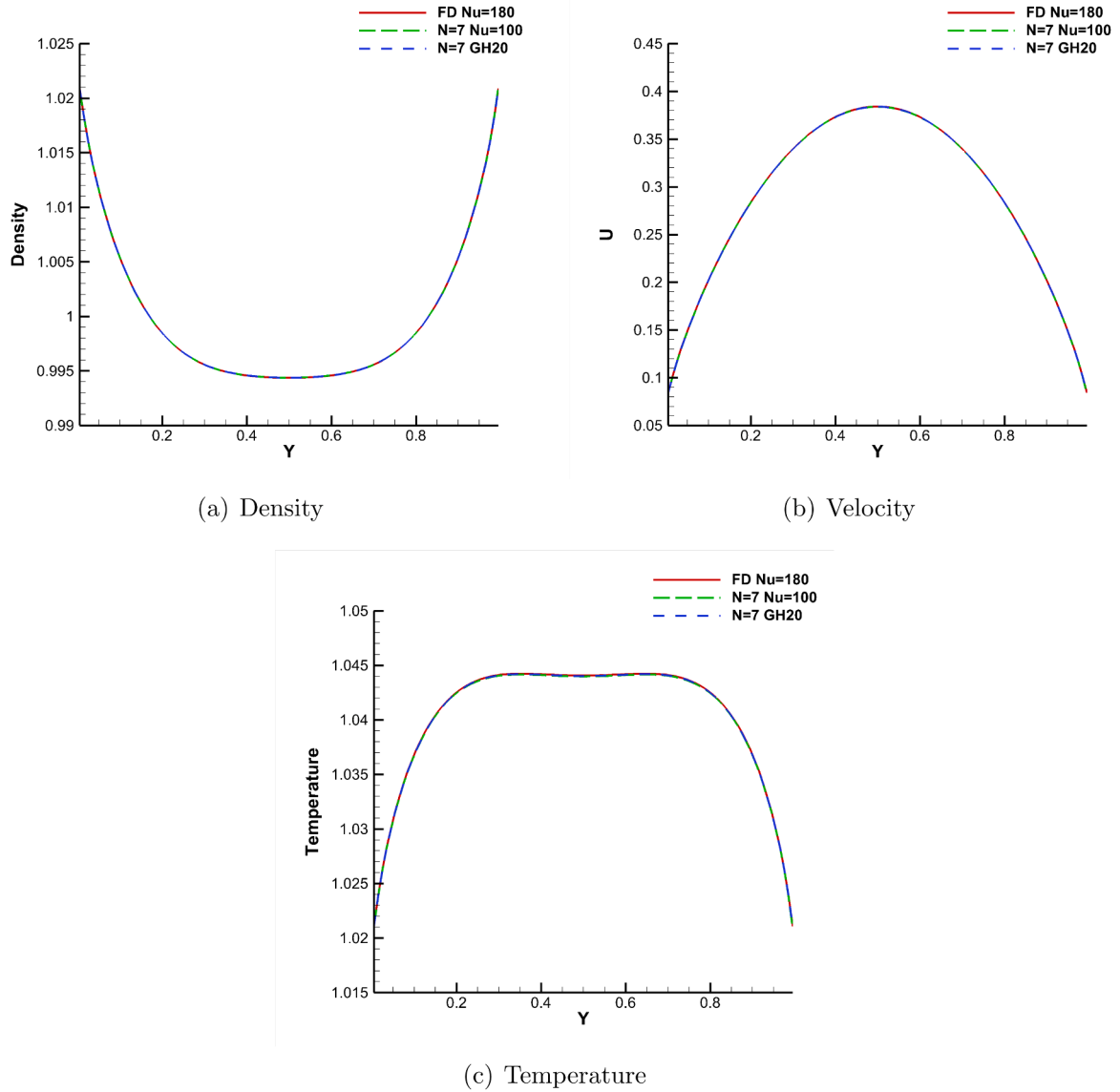


Fig. 10. Distributions of density, velocity, and temperature in the Poiseuille flow problem at $\text{Kn} = 0.1$. Here, N represents the order of the Hermite expansion, GH denotes the Gauss-Hermite quadrature, and the rest that are not specifically labeled denote the Newton-Cotes quadrature.

different magnitudes on the heat transfer at $\text{Kn} = 0.1$ is investigated. The detailed computational setup is provided in Table 6.

Fig. 8 presents the distributions of heat flux, density, and temperature under different external forces. The modulation of density by external forces is precisely captured. The non-equilibrium heat flux induced by the external force and its resulting changes in temperature profiles are quantitatively identified [6,7].

Table 7 lists the computational costs of different methods (i.e., the Hermite approximation in Section 3.3 and the second-order central difference). The results show that the Hermite spectral method, along with the Gauss-Hermite quadrature, significantly improves the computational efficiency of the numerical method at different reference Knudsen numbers. The amount of computational degrees of freedom and overall time have been reduced by 95%.

4.5. Poiseuille flow

The force-driven Poiseuille flow of rarefied gas between two infinitely parallel isothermal plates is considered. Initially stationary homogeneous gas is subjected to a constant body force acting in the posi-

Table 6

Computational setup of one-dimensional Fourier flow problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Gas	Force	x	N_x	u	N_u	Order
Argon	[0.5, 2]	[0, 1]	800	[-5, 5]	[10, 300]	2
N_m	a	Kn	Quadrature	Integrator	Boundary	CFL
[4, 10]	[0.5, 2]	[0.0001, 0.1]	NC/GH	IMEX	Dirichlet	0.5

tive x -direction parallel to the plates. The particle distribution function is initialized as Maxwellian. The detailed computational setup can be found in Table 8.

Figs. 9 and 10 present the distributions of density, velocity, and temperature at different Knudsen numbers. Table 9 lists the computational costs of different methods (i.e., the Hermite approximation in Section 3.3). It can be observed that the Hermite spectral method, along with the Gauss-Hermite quadrature, achieves a 30-fold efficiency improvement while maintaining equivalent computational accuracy. The non-equilibrium distributions of density, velocity, and temperature under wall effects are clearly identified.

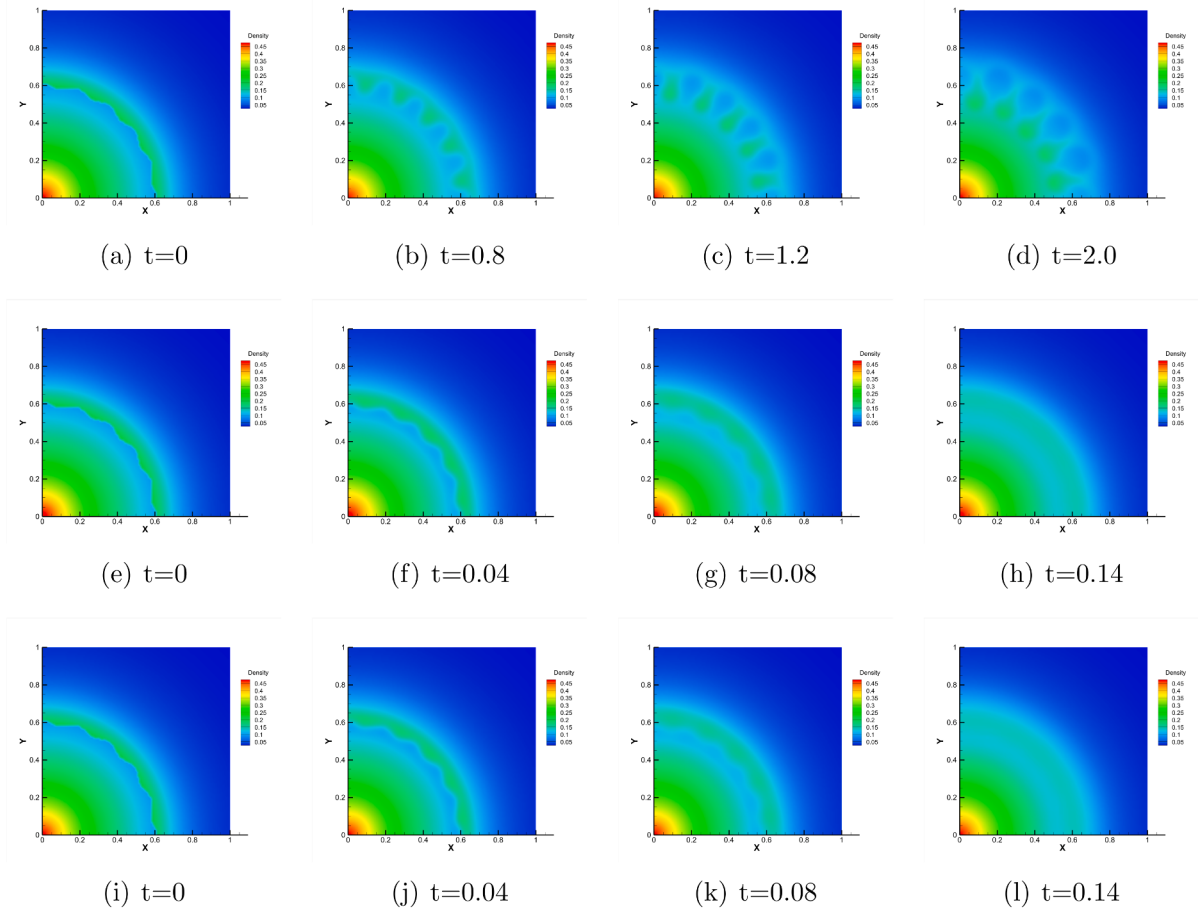


Fig. 11. Density evolution in the Rayleigh–Taylor instability problem at reference Knudsen numbers 0.0001(1st row), 0.01(2nd row), 1(3rd row).

Table 7

Computational costs of different methods for solving the one-dimensional Fourier flow problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Force	Numerical method	Number of collocation points	Time (s)
0.5	finite difference (NC)	200	5580.48
	Hermite (NC, $N_m = 4$)	80	1896.40
	Hermite (GH, $N_m = 4$)	10	263.15
1.0	finite difference (NC)	200	5999.65
	Hermite (NC, $N_m = 6$)	80	2694.69
	Hermite (GH, $N_m = 6$)	14	423.10
1.5	finite difference (NC)	300	14209.96
	Hermite (NC, $N_m = 8$)	80	2832.79
	Hermite (GH, $N_m = 8$)	18	865.73
2.0	finite difference (NC)	300	12398.12
	Hermite (NC, $N_m = 10$)	80	4785.77
	Hermite (GH, $N_m = 10$)	22	1585.94

4.6. Rayleigh–Taylor instability

The last numerical experiment is the Rayleigh–Taylor problem. The distribution of initially static gas in a two-dimensional polar coordinates (r, θ) is set as

$$\rho_0(r) = e^{-\alpha(r+r_0)}, \quad p_0(r) = \frac{1.5}{\alpha} e^{-\alpha(r+r_0)}, \quad \mathbf{V}_0 = 0, \quad (58)$$

with

$$\begin{aligned} \alpha &= 2.68, r_0 = 0.258, \quad r \leq r_1, \\ \alpha &= 5.53, r_0 = -0.308, \quad r > r_1, \end{aligned} \quad (59)$$

Table 8

Computational setup of the Poiseuille flow problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Gas	t	x	N_x	u	N_u	Order
Argon	(0, 0.2]	[0, 1]	100	$[-5, 5]$	[16, 180]	2
N_m	a	Kn	Quadrature	Integrator	Boundary	CFL
7	0.1	[0.02, 0.1]	NC/GH	IMEX	Dirichlet	0.5

Table 9

Computational costs of different methods for solving the Poiseuille flow problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Knudsen number	Numerical method	Number of collocation points	Time (s)
0.02	finite difference (NC)	140	126103.57
	Hermite (NC, $N_m = 7$)	80	41981.64
	Hermite (GH, $N_m = 7$)	16	8465.92
0.1	finite difference (NC)	180	53638.11
	Hermite (NC, $N_m = 7$)	100	17172.96
	Hermite (GH, $N_m = 7$)	20	1682.34

Table 10

Computational setup of the Rayleigh–Taylor instability problem (NC/GH refers to the Newton-Cotes/Gauss-Hermite quadrature).

Gas	t	x	N_x	y	N_y	u	N_u
Argon	(0, 2.0]	[0, 1]	120	[0, 1]	120	$[-5, 5]$	[18, 70]
v	N_v	Order	N_m	a	Kn	Quadrature	Integrator
$[-5, 5]$	[18, 70]	2	[0, 4]	-1.5	[0.0001, 1]	NC/GH	IMEX
Boundary	CFL						
Specular	0.5						

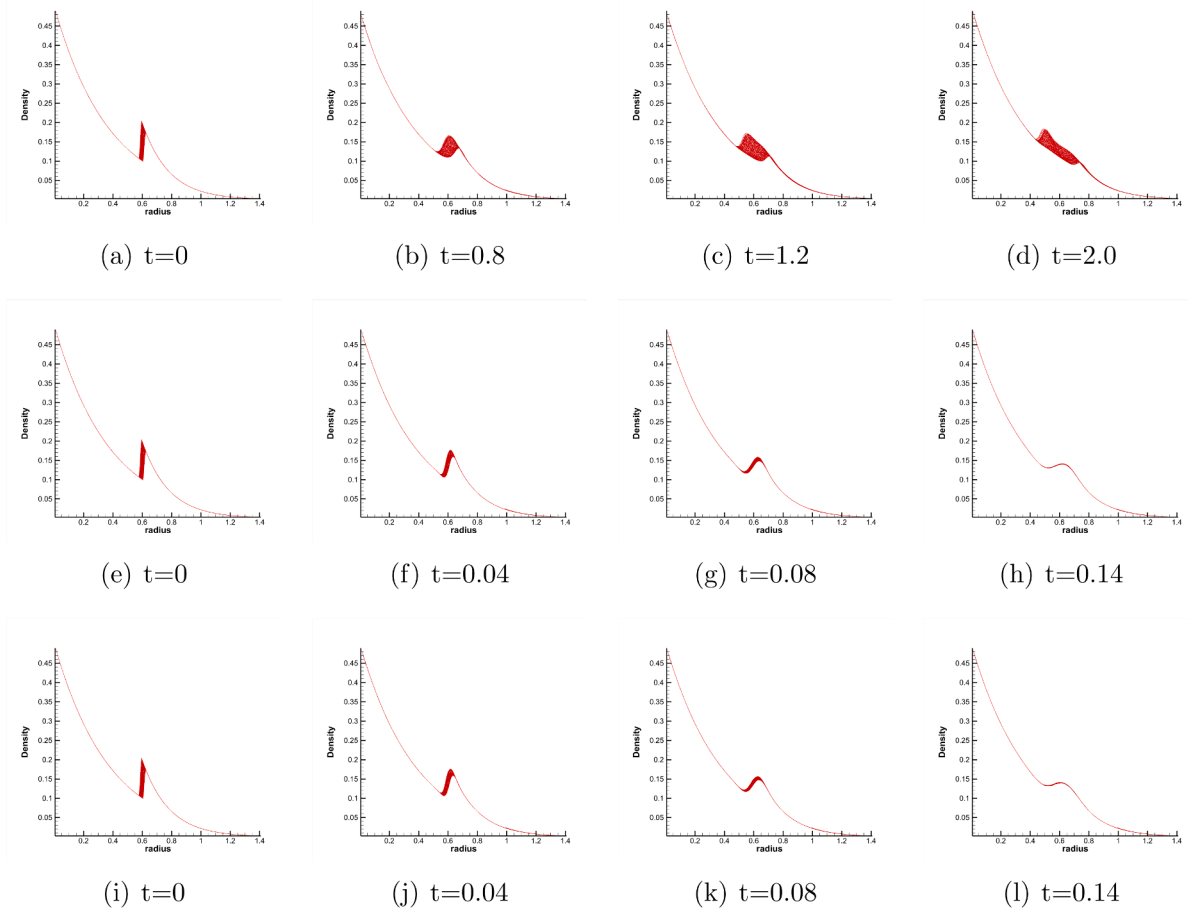


Fig. 12. Density distribution along the radial direction in the Rayleigh–Taylor instability problem at reference Knudsen numbers 0.0001(1st row), 0.01(2nd row), 1(3rd row).

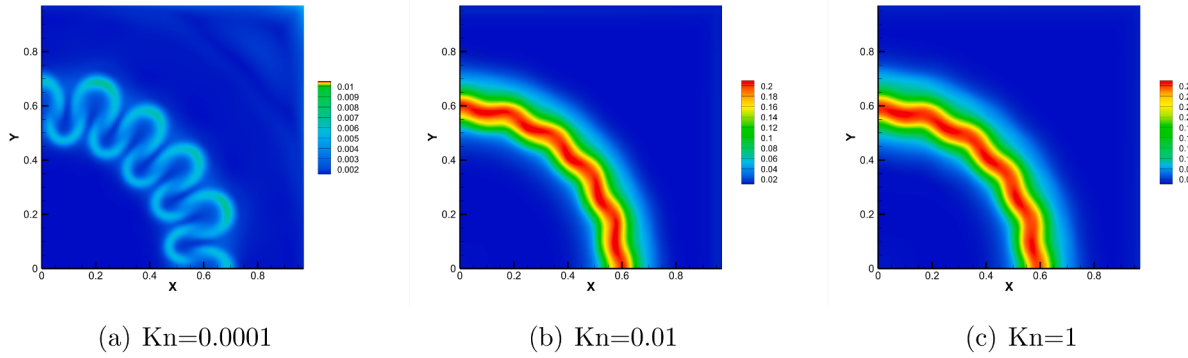


Fig. 13. The deviation of the particle distribution function from equilibrium at the final time instant in the Rayleigh–Taylor instability problem.

Table 11

Computational costs of different methods for solving the Rayleigh–Taylor problem (NC/GH refers to the Newton–Cotes/Gauss–Hermite quadrature).

Knudsen number	Numerical method	Number of collocation points	Time (s)
0.0001	finite difference (NC)	50	259314.78
	Hermite (NC, $N_m = 0$)	30	43436.27
	Hermite (GH, $N_m = 0$)	18	8926.044
0.01	finite difference (NC)	70	46080.32
	Hermite (NC, $N_m = 1$)	40	6925.77
	Hermite (GH, $N_m = 1$)	20	930.39
1	finite difference (NC)	90	176955.60
	Hermite (NC, $N_m = 4$)	50	45807.11
	Hermite (GH, $N_m = 4$)	24	3836.53

where

$$\begin{aligned} r_1 &= 0.6(1 + 0.02 \cos(20\theta)), \quad \text{for density,} \\ r_1 &= 0.62324965, \quad \text{for pressure.} \end{aligned} \quad (60)$$

The particle distribution function is initialized as Maxwellian. The detailed computational setup can be found in Table 10.

The density contours at different time instants are shown in Fig. 11. The evolution patterns of the Rayleigh–Taylor instability across varying rarefaction regimes have been identified. Within the continuum regime, as illustrated in the first panel of Fig. 11, the frequent intermolecular collisions lead to intense fluid mixing around the interface between heavy and light fluids. Conversely, increasing Knudsen number accelerates the fluid mixing process through enhanced particle transport phenomena,

thereby significantly reducing the manifestations of interfacial instability. Fig. 12 presents the density distribution in the radial direction across all elements, which provides a quantitative characterization of the mixing zone. Fig. 13 shows the degree of deviation of the distribution function away from equilibrium at the final time, defined as

$$\|f - \mathcal{M}\|_2, \quad (61)$$

where $\|\cdot\|_2$ denotes the L^2 norm. It can be observed that non-equilibrium effects are intrinsically coupled with flow patterns and scale proportionally with the degree of rarefaction. This numerical experiment again verifies the asymptotic-preserving and well-balanced properties of the solution algorithm. In all flow regimes, the hydrostatic solution is well preserved in the computation, while the mixing process only occurs near the Rayleigh–Taylor interface.

Table 11 provides the computational costs of different methods. The results demonstrate that the computational efficiency of the current method is significantly improved compared to classical discrete velocity methods while maintaining equivalent accuracy. 30- to 50-fold acceleration is achieved for the flows ranging from continuum ($\text{Kn}=0.0001$) to rarefied ($\text{Kn}=1$). The measured data validates the scalability of the solution algorithm for multi-scale flows.

5. Conclusion

This work presents a unified, Hermite-spectral-based solution algorithm for multi-scale flows under an external force grounded in the Boltzmann–BGK framework. A seamless connection between computational methods and physical models is achieved by merging a high-order Hermite spectral representation of the velocity distribution with a multi-scale evolution model inspired by the unified gas-kinetic scheme. The equilibrium and non-equilibrium flow physics across continuum and rarefied regimes are robustly coupled without sacrificing computational efficiency. The use of the spectral-collocation method not only provides spectral accuracy in the representation of non-equilibrium distribution functions, but also, through careful selection of quadrature points and weights, yields up to 50-fold acceleration compared to classical discrete velocity methods, all while preserving key physical structures such as the well-balanced hydrostatic equilibrium and correct asymptotics. Through a comprehensive suite of benchmark tests, we have demonstrated the accuracy, efficiency, and robustness of the current methodology across a wide range of Knudsen numbers and external-force magnitudes. Looking forward, the inherent flexibility of the solution algorithm offers promising avenues for extension to three-dimensional problems, complex geometries, and more generalized molecule models, paving the way for efficient, high-fidelity simulations of non-equilibrium force-driven flows in aerothermodynamics, microfluidics, astrophysics, and beyond.

CRediT authorship contribution statement

Shuangqing Liu: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation; **Zuoxu Li:** Writing – review & editing, Validation, Software, Methodology, Investigation, Formal analysis, Data curation; **Yonghao Zhang:** Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition; **Tianbai Xiao:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

Appendix A. Hermite expansion and implementation

A.1. Mathematical formulation of hermite expansion

The Hermite spectral method and the corresponding numerical scheme for approximating the particle distribution function are detailed. The Hermite polynomials are defined as

$$\mathcal{H}^{(n)}(\mathbf{u}) = \frac{(-1)^n}{\omega(\mathbf{u})} \nabla_{\mathbf{u}}^{(n)} \omega(\mathbf{u}), \quad (\text{A.1})$$

Here $\omega(\mathbf{u}) \equiv \frac{1}{\sqrt{2\pi}^D} \exp\left(-\frac{\mathbf{u}^2}{2}\right)$ with D being the dimension, and $\mathbf{u} = (\mathbf{v} - \mathbf{V})/\sqrt{RT}$ is a dimensionless measure of velocity. The recursive formulas are

$$\begin{aligned} \mathcal{H}^{(n+1)}(\mathbf{u})_{i_1 \dots i_{n+1}} &= u_{i_1} \mathcal{H}^{(n)}_{i_2 \dots i_{n+1}} - \delta_{i_1 i_2} \mathcal{H}^{(n-1)}_{i_3 \dots i_{n+1}} \\ &\quad - \delta_{i_1 i_3} \mathcal{H}^{(n-1)}_{i_2 i_4 \dots i_{n+1}} - \dots - \delta_{i_1 i_{n+1}} \mathcal{H}^{(n-1)}_{i_2 \dots i_n}, \end{aligned} \quad (\text{A.2})$$

where $\{i_1, i_2, \dots, i_{n+1}\}$ denotes the indices of a tensor, and δ is the identity tensor. Eq. (A.2) leads to

$$\begin{aligned} \mathcal{H}^{(0)}(\mathbf{u}) &= 1, \\ \mathcal{H}^{(1)}(\mathbf{u}) &= \mathbf{u}, \\ \mathcal{H}^{(2)}(\mathbf{u}) &= \mathbf{u} \otimes \mathbf{u} - \delta, \\ \mathcal{H}^{(3)}(\mathbf{u}) &= \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} - 3\mathbf{u} \otimes \delta, \\ \mathcal{H}^{(4)}(\mathbf{u}) &= \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} - 6\mathbf{u} \otimes \mathbf{u} \otimes \delta + 3\delta \otimes \delta, \\ &\dots \end{aligned} \quad (\text{A.3})$$

where the dyadic product operator leads to higher-order tensors. For example, we have

$$\mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} = u_i u_j u_k u_l, \quad (\text{A.4a})$$

$$\mathbf{u} \otimes \delta = (u_i \delta_{jk} + u_j \delta_{ik} + u_k \delta_{ij})/3. \quad (\text{A.4b})$$

For D velocity dimensions, a distribution f can be expanded within the Hermite polynomials,

$$f \approx f_{N_m} = \omega(\mathbf{u}) \sum_{n=0}^{N_m} \frac{1}{n!} \mathbf{d}^{(n)} : \mathcal{H}^{(n)}(\mathbf{u}), \quad (\text{A.5})$$

where

$$\begin{aligned} \mathbf{d}^{(n)}(t, \mathbf{x}) &= \int_{\mathbb{R}^D} f(t, \mathbf{x}, \mathbf{v}(\mathbf{u})) \mathcal{H}^{(n)}(\mathbf{u}) d\mathbf{u} \\ &= \frac{1}{(RT)^{D/2}} \int_{\mathbb{R}^D} f(t, \mathbf{x}, \mathbf{v}) \mathcal{H}^{(n)}(\mathbf{u}(\mathbf{v})) d\mathbf{v} \\ &\approx \frac{1}{(RT)^{D/2}} \sum_{j=1}^{N_v} w_j^{(\mathbf{v})} f_j \mathcal{H}_j^{(n)}. \end{aligned} \quad (\text{A.6})$$

The leading moments are

$$\mathbf{d}^{(0)}(t, \mathbf{x}) = \frac{\rho}{(RT)^{D/2}} \approx \frac{1}{(RT)^{D/2}} \sum_{j=1}^{N_v} w_j^{(\mathbf{v})} f_j, \quad (\text{A.7a})$$

$$\mathbf{d}^{(1)}(t, \mathbf{x}) = \frac{1}{(RT)^{(D+1)/2}} \int_{\mathbb{R}^D} f(\mathbf{v})(\mathbf{v} - \mathbf{V}) d\mathbf{v} = \mathbf{0}, \quad (\text{A.7b})$$

$$\mathbf{d}^{(2)}(t, \mathbf{x}) = \frac{\mathbf{T}}{(RT)^{D/2+1}} \approx \frac{1}{(RT)^{D/2}} \sum_{j=1}^{N_v} w_j^{(v)} f_j(\mathbf{u}_j \otimes \mathbf{u}_j - \delta). \quad (\text{A.7c})$$

where $\mathbf{T}$ is the modified stress defined in Eq. (35).

A.2. Numerical implementation of hermite polynomials

In the one-dimensional case, the weight function and the normalized velocity are $\omega(u) \equiv \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$, $u = (v - V)/\sqrt{RT}$. Reduced from Eq. (A.2)), the one-dimensional Hermite polynomials follow the recursion relation

$$\mathcal{H}^{(n+1)}(u) = u \mathcal{H}^{(n)}(u) - n \mathcal{H}^{(n-1)}(u), \quad n \geq 1. \quad (\text{A.8})$$

Using the definition in Eq. (A.3) and the recursive formula given in Eq. (A.8), the expansion components are derived as:

$$\begin{aligned} \mathcal{H}^{(0)} &= 1 \\ \mathcal{H}^{(1)} &= u \\ \mathcal{H}^{(2)} &= u^2 - 1 \\ \mathcal{H}^{(3)} &= u \mathcal{H}^{(2)} - 2 \mathcal{H}^{(1)} = u^3 - 3u \\ \mathcal{H}^{(4)} &= u \mathcal{H}^{(3)} - 3 \mathcal{H}^{(2)} = u^4 - 6u^2 + 3 \\ &\dots \end{aligned} \quad (\text{A.9})$$

A one-dimensional numerical implementation of the Hermite polynomials is provided to clarify the recursive structure of the basis functions and the computation of expansion coefficients.

Listing 1: Example code for one-dimensional Hermite polynomials

```

1 ! 1D Maxwellian weight at discrete
   velocities
2
3 ! Normalized velocity for Hermite
   expansion
4 u_x = (CX1D - u(1)) / dsqrt(R*T)
5 w = dexp(-0.5d0*u_x**2) / dsqrt(2.d0*PI)
6 ! Compute Hermite polynomials up to
   specified order
7 do n = 0, order
8     select case (n)
9     case (0)
10        h(0,:) = 1.d0
11     case (1)
12        h(1,:) = u_x
13     case (2)
14        h(2,:) = u_x**2 - 1.d0
15     case default
16        h(n,:) = u_x * h(n-1,:) - real(n
17        -1,8) * h(n-2,:)
18     end select
19 end do
20 ! h(n,:) stores nth-order Hermite
   polynomial values

```

In high-dimensional cases, the Hermite basis functions and their expansion coefficients can be expressed as fully indexed symmetric tensors. Due to tensor symmetry, only the independent components need to be evaluated, which substantially reduces the computational cost. In D -dimensional case, the count of independent components of a fully symmetric tensor of order N is given by a combinatorial number $\binom{N+D-1}{N}$. For example, in two dimensions the number is $N+1$, while in three dimensions it is $(N+1)(N+2)/2$.

To illustrate this result, we first consider the two-dimensional case. A symmetric tensor of order n can be expressed in compact form.

$$\mathcal{H}_{x^r y^s}^n, \quad r + s = n, \quad (\text{A.10})$$

where the multiplicity of each component is given by the binomial coefficient $\binom{n}{r}$. For example,

$$\mathcal{H}_{xxy} = \mathcal{H}_{yyx} = \mathcal{H}_{yxy} \equiv \mathcal{H}_{xy^2}. \quad (\text{A.11})$$

This representation naturally extends to three-dimensional case. A symmetric tensor of order n can be written as

$$\mathcal{H}_{x^r y^s z^t}^n, \quad r + s + t = n, \quad (\text{A.12})$$

where the multiplicity of each component is determined by the trinomial coefficient $\frac{n!}{r!s!t!}$. This compact notation highlights the redundancy reduction achieved by exploiting tensor symmetry and will be adopted in the following derivations for clarity and efficiency.

For two dimensional situation, $\omega(\mathbf{u}) \equiv \frac{1}{2\pi} \exp\left(-\frac{\mathbf{u}^2}{2}\right)$, $u_x = (v_x - V_x)/\sqrt{RT}$ and $u_y = (v_y - V_y)/\sqrt{RT}$. Using the definition in Eq. (A.3) and the recursive formula given in Eq. (A.2), the expansion components are defined as

$$\text{1st order: } \mathcal{H}_x^{(1)} = u_x,$$

$$\mathcal{H}_y^{(1)} = u_y,$$

$$\text{2nd order: } \mathcal{H}_{x^2}^{(2)} = (\mathcal{H}_x^{(1)})^2 - 1 = u_x^2 - 1,$$

$$\mathcal{H}_{xy}^{(2)} = \mathcal{H}_x^{(1)} \mathcal{H}_y^{(1)} = u_x u_y,$$

$$\mathcal{H}_{y^2}^{(2)} = (\mathcal{H}_y^{(1)})^2 - 1 = u_y^2 - 1,$$

$$\text{3rd order: } \mathcal{H}_{x^3}^{(3)} = \mathcal{H}_x^{(1)} \mathcal{H}_{x^2}^{(2)} - 2 \mathcal{H}_x^{(1)} = u_x^3 - 3u_x,$$

$$\mathcal{H}_{x^2 y}^{(3)} = \mathcal{H}_x^{(1)} \mathcal{H}_{x^2 y}^{(2)} - \mathcal{H}_y^{(1)} = u_x^2 u_y - u_y,$$

$$\mathcal{H}_{x y^2}^{(3)} = \mathcal{H}_x^{(1)} \mathcal{H}_{y^2}^{(2)} = u_x u_y^2 - u_x,$$

$$\mathcal{H}_{y^3}^{(3)} = \mathcal{H}_y^{(1)} \mathcal{H}_{y^2}^{(2)} - 2 \mathcal{H}_y^{(1)} = u_y^3 - 3u_y,$$

$$\text{4th order: } \mathcal{H}_{x^4}^{(4)} = \mathcal{H}_x^{(1)} \mathcal{H}_{x^3}^{(3)} - 3 \mathcal{H}_{x^2}^{(2)} = u_x^4 - 6u_x^2 + 3,$$

$$\mathcal{H}_{x^3 y}^{(4)} = \mathcal{H}_x^{(1)} \mathcal{H}_{x^2 y}^{(3)} - 2 \mathcal{H}_{xy}^{(2)} = u_x^3 u_y - 3u_x u_y,$$

$$\mathcal{H}_{x^2 y^2}^{(4)} = \mathcal{H}_x^{(1)} \mathcal{H}_{x y^2}^{(3)} - \mathcal{H}_{y^2}^{(2)} = u_x^2 u_y^2 - u_x^2 - u_y^2 + 1,$$

$$\mathcal{H}_{x y^3}^{(4)} = \mathcal{H}_x^{(1)} \mathcal{H}_{y^3}^{(3)} = u_x u_y^3 - 3u_x u_y,$$

$$\mathcal{H}_{y^4}^{(4)} = \mathcal{H}_y^{(1)} \mathcal{H}_{y^3}^{(3)} - 3 \mathcal{H}_{y^2}^{(2)} = u_y^4 - 6u_y^2 + 3,$$

...

For clarity, a two-dimensional numerical implementation of the Hermite polynomials is provided to illustrate the recursive structure of the basis functions.

Listing 2: Source code for the two-dimensional Hermite expansion

```

1 ! 2D Maxwellian weight at discrete
   velocity points
2
3 ! Normalized velocities for Hermite
   expansion
4 u_x = (CX2D - u(1)) / dsqrt(R*T)
5 u_y = (CY2D - u(2)) / dsqrt(R*T)
6 w = dexp(-0.5d0*(u_x**2 + u_y**2)) / (2.
   d0*PI)
7 ! Compute 2D Hermite polynomials up to
   specified order
8 do n = 0, order

```

```

9      do i = 0, n
10         j = n - i
11         select case (n)
12         case (0)
13             h(0,0,,:) = 1.d0
14         case (1)
15             if (i == 1) h(1,0,,:) = u_x
16             if (j == 1) h(0,1,,:) = u_y
17         case (2)
18             if (i == 2) h(2,0,,:) = u_x
19                 **2 - 1.d0
20             if (i == 1 .and. j == 1) h
21                 (1,1,,:) = u_x * u_y
22             if (j == 2) h(0,2,,:) = u_y
23                 **2 - 1.d0
24         case default
25             if (j == 0 .and. i >= 2)
26                 then
27                     h(i,0,,:) = u_x * h(i
28                         -1,0,,:) - real(i
29                         -1,8) * h(i-2,0,,:)
30                 else if (i == 0 .and. j >=
31                     2) then
32                     h(0,j,,:) = u_y * h(0,j
33                         -1,,:) - real(j-1,8)
34                         * h(0,j-2,,:)
35                 else if (i >= 2) then
36                     h(i,j,,:) = u_x * h(i
37                         -1,j,,:) - real(i
38                         -1,8) * h(i-2,j,,:)
39                 else
40                     h(1,j,,:) = u_x * h(0,j
41                         ,,:) ! i=1, j>=1
42             end if
43         end select
44     end do
45 end do
46
47 ! h(i,j,,:) stores the polynomial of
48 order i in x and j in y

```

By the independent component denotation of symmetric tensors, the forcing term can be further simplified. We define $\mathbf{b}^{(n+1)} = \text{Sym}(\mathbf{a} \otimes \mathbf{d}^{(n)})$, where the normalized symmetrization is

$$b_{i_0 i_1 \dots i_n}^{(n+1)} = \frac{1}{n+1} \sum_{k=0}^n a_{i_k} d_{i_0 \dots \hat{i}_k \dots i_n}^{(n)}.$$

In the one-dimensional case, we have

$$a \partial_v f_{N_m} = -\frac{\omega(u)}{\sqrt{RT}} \sum_{n=0}^{N_m} \frac{1}{n!} b^{(n+1)} H^{(n+1)}(u). \quad (\text{A.14})$$

which becomes

$$\mathbf{a} \cdot \nabla_v f_{N_m} = -\frac{\omega(\mathbf{u})}{\sqrt{RT}} \sum_{n=0}^{N_m} \sum_{r=0}^{n+1} \frac{n+1}{r! s!} b_{x^r y^s}^{(n+1)} \mathcal{H}_{x^r y^s}^{(n+1)}. \quad (\text{A.15})$$

for the two-dimensional case, where $s = n+1-r$. In the three-dimensional case, it becomes

$$\mathbf{a} \cdot \nabla_v f_{N_m} = -\frac{\omega(\mathbf{u})}{\sqrt{RT}} \sum_{n=0}^{N_m} \sum_{r=0}^{n+1} \sum_{s=0}^{n+1-r} \frac{n+1}{r! s! t!} b_{x^r y^s z^t}^{(n+1)} \mathcal{H}_{x^r y^s z^t}^{(n+1)}. \quad (\text{A.16})$$

where $t = n+1-r-s$.

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