Kinetic Node-Pair Formulation for Two-Dimensional Flows from Continuum to Transitional Regime

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A hybrid finite-element/finite-volume node-pair discretization of conservation laws is reformulated in terms of a Bhatnagar–Gross–Krook kinetic scheme to address flows from the continuum up to the transitional regime in a seamless fashion. Integrals of the particle distribution function from the kinetic theory of gases are adopted to compute the numerical fluxes along the boundary of each control volume. Flow features typical of the transitional regime like velocity and temperature slip condition at solid walls are automatically assured by the kinetic formulation of the node-pair boundary conditions. Exemplary two-dimensional numerical experiments ranging from continuum flows up to the transitional regime are presented.

I. Introduction

The simultaneous existence of different flow regimes is a condition that characterizes the aerothermodynamics of many aircraft and space vehicles. Examples of this condition are the early atmospheric flight during the entry phase of a space vehicle, the flow regimes of aircraft designed to cruise at hypersonic speeds, or the operating conditions of some propulsive systems intended to work in a very rarefied environment. The presence of strong shock waves, large separation, recirculation zones, strong rarefactions and/or a general low-density level due to the high altitudes are all elements that determine a complex scenario where regions of local or quasi-local equilibrium flow coexist and merge with areas where the continuum hypothesis and the assumption of an equilibrium state are lost up to the level where, for some extreme conditions, a free molecular regime is established.

Being intermediate between the continuum state and the free molecular flow, the transitional regime is identified by values of the Knudsen number (Kn) up to unity. At these values of Kn, classical models and numerical methods based on the macroscopic continuum-based Navier–Stokes equations are not applicable due to the sensible role played by nonlocal effects. At the same time, the mild level of rarefaction causes numerical difficulties in the adoption of the standard particle-based methods [1,2]. In this case, in fact, the computational expense required to simulate the relatively high number of particles typical of this regime poses serious limits to the practicality of the approach. In other words, in the transitional regime, well-established methods of computational fluid dynamics may fail because of either crude physical modeling or excessive computational cost.

In the realm of the macroscopic formulations, the standard approach to the simulation of transitional flows is to force the supposed nonequilibrium effects inside the mathematical and numerical models. Typically, this is obtained by specifying enhanced transport properties, very complicated macroscopic conservation equations, and/or explicitly enforcing velocity/temperature slip conditions at solid walls [3–7]. The mathematical and numerical complexity and, in some cases, the lack of a solid theoretical background pose serious limits to the general adoption of these methods for realistic problems [8]. A more sophisticated approach is instead represented by hybrid methodologies that, on one hand, use a macroscopic continuum-based approach where the flow is assumed to be in a quasi-equilibrium state, but on the other side they recur to...
particle-based methods to model areas where the equilibrium condition is lost. Simplicity and numerical robustness has made hybrid approaches quite popular in the recent literature [9–13]. Nevertheless, significant drawbacks can be recognized. First of all, this technique requires the definition of a suitable domain-decomposition method to discriminate between equilibrium and nonequilibrium regions. Second, the definition of a method to exchange information at the frontier between the two regions is a nontrivial problem. In fact, the two methods rely on completely different formulations. On one side, there is a macroscopic formulation that provides fairly smooth and regular representations of the flow. On the other side, there is the microscopic approach that is typically affected by noisy and scattered distributions. Even if specific methods have been developed to put a remedy to this problem [14], moving from one description to another introduces numerical errors that eventually affect the accuracy of the solution.

A valid alternative to the cited methodologies is represented by the so-called kinetic schemes [15–19]. Such schemes can be regarded as a blend of the macroscopic and particle-based methods because they explicitly adopt elements of the kinetic theory of gases in the framework of a macroscopic formulation of the conservation laws. This characteristic makes them appealing from both a physical and numerical point view. In fact, first of all, they are built on the solid theoretical base of the kinetic theory of gases that is valid for any flow regime. Second, this approach provides unified discrete formulations that avoid the necessity of communicating between different methods. As a result, the kinetic schemes open the way to numerical methods that can be applied effectively and efficiently on a wide range of flow regimes.

In the context of the kinetic schemes based on the Bhatnagar–Gross–Krook (BGK) model of the Boltzmann equation, Xu [20] proposed a method to address both continuum (quasi-equilibrium) and transitional (nonequilibrium) flows on the basis of an accurate description of the collision process of the particles of the gas. In fact, by introducing high-order terms of the Chapman–Enskog expansion [21] directly in the definition of the collision frequency between molecules [22], different regimes can be addressed by virtue of the same mathematical and numerical models for continuum flows. Namely, Xu [20] uses a first-order closure of the Chapman–Enskog expansion with a novel definition of the mean collision time that accounts for high-order effects. In this way, the nonequilibrium conditions are ultimately represented as a rather simple and efficient modification of the classical transport properties of the gas. The so-called kinetic-BGK method of Xu has been successfully adopted in the framework of many standard finite-volume formulations for conservation laws [23–26] based either on fully structured or fully unstructured meshes made of triangles/tetrahedra [27–29], adopting implicit and/or explicit formulations [30]. Recently, fundamental and applied researches have appeared in literature that propose the application of such a scheme in the context of discontinuous Galerkin finite-element discretizations [31,32].

The present work describes the reformulation of the so-called node-pair discretization of the flow equations [33,34] on the basis of the kinetic-BGK scheme proposed by Xu [20,35]. Two aspects of the numerical simulation of continuum-transitional flows will then be addressed with the present node-pair–BGK scheme. The first one is the ability to model equilibrium and nonequilibrium flows in a unified and seamless manner, and this is guaranteed by the adoption of a kinetic scheme. The second aspect concerns the capability to handle efficiently the potentially complex geometries of modern air space-craft. In this sense, the node-pair formulation allows operation on grids made of elements of different topology in an efficient and unified fashion via the adoption of unstructured hybrid meshes and mesh-adaptation techniques. The node-pair formulation is also significant for its ability to state equivalence conditions between finite-volume and finite-element formulations [34]. Nevertheless, the discussion of this equivalence properties with respect to the kinetic scheme-BGK is out the scope of the present paper, and it is left to a future investigation.

The discussion is organized as follows. In Sec. II, the basics of the node-pair discretization will be introduced together with a novel formulation of the interface fluxes that will allow the introduction the BGK scheme. In Sec. III, the BGK kinetic scheme will be introduced, and the mathematical and numerical details of its inclusion in the node-pair framework will be addressed both in the cases of continuum and transitional regimes. Section IV will present an overview of the kinetic treatment of the boundary conditions, and eventually Sec. V will present some numerical experiments.

II. Node-Pair Discretization of the Finite-Volume Approach

Let us consider a median dual tessellation over a two-dimensional domain $\Omega$. For each control volume $C_i$, the integral form of the system of conservation laws reads

$$\frac{d}{dt} \int_{C_i} w = - \int_{\partial C_i} j \cdot n \quad \forall \, C_i \subseteq \Omega \quad (1)$$

where $w$ is a $\mathbb{R}^d$ vector collecting the conserved variables, $j$ is the $\mathbb{R}^d \times \mathbb{R}^d$ hypervector of the fluxes with spatial components, $n = (n_1, n_2)$, each of which is a vector of $\mathbb{R}^d$, and $n$ indicates the outward normal versor of the control volume $C_i$.

The node-pair structure emerges as the right-hand side of Eq. (1) is rearranged in a form in which the fluxes across the interface of $C_i$ are rewritten as the sum of the contributions associated to each couple of nodes issuing from the node $i$. Splitting the contributions of the node pairs inside the domain and the contributions of the couple of nodes lying on the boundary, the right hand side of Eq. (1) reads

$$\int_{\partial C_i} j \cdot n \cong \sum_{k \in \mathcal{K}_{i,d}} J_{ik} \cdot n_k + \sum_{e \in \mathcal{E}_i^I} \mathcal{J}_e^{i,e} \cdot v_e^{i,e} \quad (2)$$

$\mathcal{K}_{i,d}$ is the set of nodes adjacent to the node $i$, and $J_{ik} = J(w_i, w_k)$, a suitable integrated numerical flux function at the $k$th interface $i-k$ that depends on the values of the conserved variables $w_i$ and $w_k$ at the two nodes of the pair; see Fig. 1. $\mathcal{E}_i^I$ is the set of elements of the boundary grid (in $\mathbb{R}^{d-1}$) defined as the intersection of the interface with the boundary of the domain $\partial \Omega$ (Fig. 2). $\mathcal{J}_e^{i,e}$ is a suitable flux function at the boundary defined as

$$\mathcal{J}_e^{i,e} \equiv J(w_e^{i,e}(s)) = \text{constant} \quad \forall \, s \in \partial C_i^{i,e} \quad (3)$$

where $w_e^{i,e}$ is the vector of conserved variables at the boundary, to be determined on the basis of the type of boundary condition selected.
Finally, \( \eta_k \) and \( \nu^{\theta \psi} \) are referred to as the integrated normal vectors and are defined as

\[
\eta_k = \int_{\partial C_k} n_i \quad \text{and} \quad \nu^{\theta \psi} = \int_{\partial C_k} n_i^r
\]

where \( \partial C_k \) is the intersection between the boundaries of the cell \( C_k \) and the cell \( C_i \), and \( \partial C_k \) is the intersection between the boundary of \( C_k \), the boundary of the computational domain \( \partial \Omega \), and the boundary of the subelement \( \Omega_i^c \) of the finite-element triangulation (Fig. 2).

### A. Domain Integrals

Each domain contribution under the first summation symbol in Eq. (2) can be computed by means of many different methods; nevertheless, this form does not allow for a straightforward formulation in terms of a BGK flux. For reasons that will become more evident in Sec. III, each term \( J_{ik} \cdot \eta_k \) is now rewritten to have the component of the fluxes along the direction of the integrated normal \( \eta_k \) explicitly appearing in the discrete equations. To this purpose, let us introduce a local reference frame having the x axis aligned with the integrated normal \( \eta_k \). The k\textsuperscript{th} domain term can then be written as follows:

\[
J_{ik} \cdot \eta_k = R^{-1}_k (J^R_{ik} \cdot \eta_k^R) \tag{5}
\]

where \( R_k \) is the rotation matrix, \( J^R_{ik} \) is the hypervector of the fluxes in the local frame, and \( \eta_k \) is the integrated normal in the rotated frame. Because the local frame is such that the x axis is aligned with the integrated normal \( \eta_k \), the vector \( \eta_k \) reads

\[
\eta_k^R = R_k \eta_k \tag{6}
\]

where \( R_k \) is the versor of the x axis in the local frame. Substituting Eq. (6) in Eq. (5) results in

\[
R^{-1}_k (J^R_{ik} \cdot \eta_k^R) = R^{-1}_k (J^R_{ik} \cdot \eta_k^R) R_k |\eta_k| \tag{7}
\]

where \( J^R_{ik} \cdot \eta_k^R \) is the desired component of the interface fluxes aligned with the normal \( \eta_k \). In the following, for ease of notation, the shortcut notation \( J_i \) will be used as an alternate expression for the k\textsuperscript{th} flux \( J^R_{ik} \).

### B. Boundary Integrals

Similar to the domain term, in the case of the boundary flux, the component of the fluxes aligned with the integrated normal \( \nu^{\theta \psi} \) has to be made explicit from each k\textsuperscript{th} term \( J_k \cdot \nu_k \). A local frame with the x axis aligned with the integrated normal \( \nu_k \) is introduced as indicated in Fig. 2, and the k\textsuperscript{th} boundary integral is eventually recast as follows:

\[
J_k \cdot \nu_k^{\theta \psi} = R^{-1}_k (J^R_{ik} \cdot \eta_k^R) \tag{8}
\]

where \( R_k \) is the boundary rotation matrix at node \( i \).

### C. Semidiscrete Form of the Conservation Laws

Approximating the vector \( w \) in each control volume \( C_i \) by means of its cell average \( w_i \),

\[
w(x, t) \approx w_i = \frac{1}{|C_i|} \int_{C_i} w \quad \forall \ x \in C_i \tag{9}
\]

and using Eqs. (7,8) for the fluxes along the boundary of the control volumes, the semidiscrete form of the conservation equations under the node-pair formulation reads

\[
|C_i| \frac{dw_i}{dt} = - \sum_{n \in S_i^C} R^{-1}_i \Delta r_{ik} |\eta_k| - \sum_{n \in Y_i^C} R^{-1}_i \Delta r_{ik} |\nu_k^{\theta \psi}| \tag{10}
\]

Equation (10) is valid regardless of the topology of the grid. In fact, any information about the type of the elements of the geometric discretization is enclosed in the two vectors \( \eta_k \) and \( \nu^{\theta \psi} \), which are referred to as metric coefficients [36,37]. When the mesh does not change with time, these coefficients can be computed once for all at the beginning of the simulation with great savings in computational time.

### III. Bhatnagar–Gross–Krook Kinetic Formulation of the Node-Pair Interface Flux

In the attempt to obtain a formulation that allows for a seamless description of the flow from continuum to transitional regime, the kinetic theory of gases is here adopted to compute the numerical fluxes for the domain and the boundary term. Given the fundamental particle distribution function \( f = f(x, t, u, \xi) \), the fluxes of the conserved quantities for any equilibrium condition and state of the gas are defined as [22]

\[
\int(u \cdot n) w f \, du \, d\xi \tag{11}
\]

where \( u \) and \( \xi \) are the velocities and the internal degrees of freedom, respectively, of the molecules of the gas, and \( w \) is a vector of functions [22] of \( u \) and \( \xi \) that are conserved during the collisions between the molecules. The form of these functions is known from the theory of gases [22], and these are usually referred to as the collisional invariants. Eventually, \( n \) is the unit vector indicating the direction along which the fluxes are required.

The particle-distribution function is obtained from the solution of the Boltzmann integro-differential equation, and its integration over the space of molecular velocities gives the mass, momentum, and total energy of the gas at each point \( x \) and at any instant of time \( t \). Because of the mathematical complexity of the Boltzmann equation and the extreme difficulty to obtain (analytically or numerically) a solution for any node and at any instant of time, approximate forms of the Boltzmann equation have been introduced to obtain \( f \) at the boundary of a generic control volume [35,38]. Following the original work of Prendergast and Xu [18] and Xu and Prendergast [19], the particle distribution can be obtained as the solution of the more tractable BGK model of the Boltzmann equation [39]. In particular, in the context of a node-pair finite-volume approximation, the computation of \( f \) at the cell interface requires the solution of the following Riemann problem:

\[
\begin{aligned}
\frac{df}{dt} + \nabla f &= f_0 - f \\
\frac{df}{dt} + \nabla f &= f_0(x, u, \xi) \times < 0 \\
\frac{df}{dt} + \nabla f &= f_0(x, u, \xi) \times > 0
\end{aligned} \tag{12}
\]

where \( x \) the direction of the integrated normal \( \eta_k \) in the case of the domain integral and the direction of \( \nu^{\theta \psi} \) in the case of the boundary term. In Eq. (12), the symbol \( f_0 \) is adopted to represent the Maxwellian equilibrium to which the gas is driven by molecule collisions, and \( r \) indicates the characteristic time of such an idealized relaxation process. The Maxwellian state is defined as

\[
f_0 = \rho \frac{\partial}{\partial x} \left( e^{-\theta[(u-U)(u-U)+\xi]} \right) \tag{13}
\]

where \( \rho \) and \( U \) are the macroscopic density and velocity, respectively; \( \theta \) is a function of temperature, molecule mass, and Boltzmann constant \( \xi \); and \( K \) is the dimension of the vector \( \xi \), which is the number of thermal degrees of freedom of the molecules. The functions \( f_1 \) and \( f_2 \) that define the initial condition of the Riemann problem represent the particle functions at the two nodes of the pair. The Riemann problem in Eq. (12) is formulated along the direction of the integrated normals, and this circumstance represents the motivation for which the node-pair semidiscrete equation has been rewritten in terms of local reference frames at each node pair.
The Riemann problem in Eq. (12) has to be solved at each (pseudo-) time step of the simulation and for each pair of interacting nodes to get the appropriate flux by which, in turn, the fluxes are obtained. An analytical solution for this problem can be found [35,38], which can be adopted in the computation, i.e.,

\[
\begin{align*}
  f(0, t, u, \mathbf{\xi}) &= \frac{1}{\tau} \int_{0}^{t} f_{0}(x', t', u, \mathbf{\xi}) e^{-(t-t')/\tau} \, dt' \\
  &+ e^{-t/\tau} f(-u, 0, u, \mathbf{\xi})
\end{align*}
\]  

(14)

where \(x' = -u(t-t')\) is the trajectories of the particles. The fundamental quantities are defined explicitly to have \(f\) at the cell interface are the two initial left and right states \(f_{L}\) and \(f_{R}\), the characteristic mean collision time \(\tau\), and a suitable intermediate macroscopic state \(\mathbf{w}_{i}\) by which the Maxwellian function in the integral relaxation term at right-hand side of Eq. (14) can be obtained.

The intermediate state is computed by applying the so-called compatibility condition to Eq. (14) in the limit of \(t \rightarrow 0\). Such a condition reads

\[
\int \frac{1}{\tau} \psi(f_{0} - f) = 0
\]

(15)

where \(\psi\) is the vector of the collisional invariants, i.e., \([1, u, 0.5(u \cdot u + \mathbf{\xi} \cdot \mathbf{\xi})]\) [22]. Equation (15) states the strict conservation of mass momentum and energy at the interface [40,41]. The mathematical details of how this constraint allows definition of an intermediate state at the cell interface can be found in the literature [35,38] and will not be reported here.

The computation of \(f_{L}\) and \(f_{R}\) is done following the fundamental work of Chapman and Enskog [21] and the work of Xu [20,35], where a first-order expansion in \(\tau\) can be adopted to approximate the left and right states in a way that both continuum and transitional regimes can be addressed.

### A. Continuum Regimes

It is well known that, in the continuum regimes, the state of the gas can be effectively addressed in terms of small departures from the equilibrium state described by the Maxwellian distribution function [21,22]. In this case, the left and right states of the Riemann problem [Eq. (12)] will then be written as [35]

\[
\begin{align*}
  f_{L} &= f_{0}^{L} - \tau D f_{0}^{L} \\
  f_{R} &= f_{0}^{R} - \tau D f_{0}^{R}
\end{align*}
\]  

(16)

where \(f_{0}^{L}\) and \(f_{0}^{R}\) are the Maxwellians corresponding to the known macroscopic quantities at the left and right states of the interface, and the symbol \(D\) refers to the combination of temporal and spatial differential operators

\[
D \equiv \frac{\partial}{\partial t} + u \cdot \nabla
\]

where \(u\) is the velocity of the molecules of the gas.

The mean collision time \(\tau\) adopted for the linearization of \(f\) is a measure of how fast the gas will reach the Maxwellian equilibrium state as a consequence of the collision process. In the classical macroscopic continuum framework, the relaxation mechanism is represented via the introduction of momentum and energy-diffusion processes controlled by the viscosity and the thermal conductivity of the fluid. In the present BGK model, to keep consistency with the macroscopic representation, the mean collision time is directly obtained from the viscosity of the gas evaluated at the same intermediate state used to compute \(f_{0}\) in Eq. (14)

\[
\tau = \frac{\mu}{P}
\]

(17)

Because thermal conductivity does not appear explicitly in Eq. (17), only fluids having a unit Prandtl number can be addressed. A remedy to this limitation has been proposed by Xu [35] and will also be adopted in the present formulation.

### B. Stencil for the Node-Pair Bhatnagar–Gross–Krook Scheme

From a computational point of view, the adoption of Eq. (16) requires the computation of the gradient of the macroscopic quantities at the two sides of the cell interface [38]. The gradients at the left and right sides of the interface are obtained on the basis of a finite-difference approximation involving the values of the macroscopic quantities in correspondence of a suitable set of nodes around the interface. In the original formulation of the node-pair discretization [34], a quasi-one-dimensional stencil is considered to obtain the gradients in the direction normal to the interface; see Fig. 3 (top). To obtain a genuine multidimensional node-pair–BGK scheme, the original stencil has been extended to account for the derivatives in the direction tangent to the integrated normal at interface. According to the topology of the grid, different approaches to select the points to be used in the finite-difference formula have been adopted. For two-dimensional problems, in the case of unstructured grids of triangles, the nodes in the tangent direction have been chosen as the ones belonging to the two triangles that contain the nodes \(i\) and \(k\); see Fig. 3 (bottom left). On the other hand, in the case of quadrilateral elements, the relevant nodes are the ones associated to the edges most aligned with the tangent direction; see Fig. 3 (bottom right). The extension of the stencil in the case of three spatial dimensions can be obtained on the basis of the same considerations adopted for the two-dimensional case.

### C. Transitional Regimes

The transitional regime is characterized by a departure from the local equilibrium condition for which an approximation of first order in \(\tau\) is not adequate, and it becomes necessary to include terms of higher order in the Chapman–Enskog expansion. Because of the early nonequilibrium conditions, approximations that include quadratic terms in \(\tau\) are usually adopted, like Burnett’s model [3]. Different from that class of methods that are derived directly from high-order closures, Xu [20] proposed to generalize the kinetic method based on a first-order expansion by introducing a modified, or regularized, formula for the computation of the mean collision time [20]. Represented here with the symbol \(\tau^{*}\), the transitional counterpart of the collision time can be obtained as a function of \(\tau\), the first-order terms, \(Df_{0}\), and the second-order terms of the Enskog expansion \(D^{2}f_{0}\), i.e.,

\[
\tau^{*} = \tau^{*}(\frac{\mu}{P}, Df_{0}, D^{2}f_{0}) = \frac{\tau}{1 + \tau((D^{2}f_{0})/(Df_{0}))}
\]

(18)

where \(\tau\) is computed as in Eq. (17), i.e., as in the case of a quasi-equilibrium assumption [35,38], and where the second-order differential operator \(D^{2}\) is computed as

![Fig. 3 Original quasi-one-dimensional stencil (top) and proposed stencil for a genuine kinetic multidimensional approach (bottom).](image-url)
\[ D^2 \equiv \frac{\partial^2}{\partial t^2} - 2a \cdot \frac{\partial}{\partial t} \nabla + u \cdot u' \] (19)

is the hessian matrix of the function to which the operator is applied, and \( \langle Df_0 \rangle \) and \( \langle D^2 f_0 \rangle \) are computed as

\[ \langle Df_0 \rangle = \int \psi \langle Df_0 \rangle \]
\[ \langle D^2 f_0 \rangle = \int \psi \langle D^2 f_0 \rangle \]

with \( \psi = (u - U)^2 \) as indicated in the literature [26]. A BGK kinetic scheme for the transitional regime is eventually obtained by adopting the regularized formula for \( \tau^* \) to define the left and right initial states of the Riemann problem [Eq. (12)]:

\[ f_L = f_0^L - \tau^* Df_0^L \quad \text{and} \quad f_R = f_0^R - \tau^* Df_0^R \] (20)

The scheme based on Eqs. (18,20) preserves the simplicity and robustness of the approaches based on first-order closures but goes beyond the limits of continuum-based methods thanks to the second-order terms \( D^2 f_0 \). In the continuum limit, the previous formulation approaches the Navier–Stokes solutions because the term \( \tau^*(D^2 f_0)/(Df_0) \) goes to zero. However, the Navier–Stokes solutions are not reproduced exactly because the correction term vanishes only when \( D^2 f_0 = 0 \).

### D. Second-Order Derivatives of the Maxwellian

To complete the description of the numerical method, it is still necessary to define a way to compute the terms appearing in \( D^2 f_0 \). Resorting to a one-dimensional description for ease of notation, the differential operators in the extended formula for \( \tau^* \) (i.e., \( Df_0 \) and \( D^2 f_0 \)) reduce to the following:

\[ Df_0 = \frac{\partial f_0}{\partial t} + u \frac{\partial f_0}{\partial x} \]
\[ D^2 f_0 = \frac{\partial^2 f_0}{\partial t^2} - 2u \frac{\partial^2 f_0}{\partial t \partial x} + u^2 \frac{\partial^2 f_0}{\partial x^2} \] (22)

The spatial and temporal derivatives of the Maxwellian can be expressed in terms of the Taylor series expansion of \( f_0 \) [38]:

\[ \frac{\partial f_0}{\partial t} = A(\psi)f_0 \quad \frac{\partial f_0}{\partial x} = a(\psi)f_0 \] (23)

where

\[ a(\psi) = a_1 + a_2 u + a_3 \frac{1}{2} (u^2 + \xi^2) \]
\[ A(\psi) = A_1 + A_2 u + A_3 \frac{1}{2} (u^2 + \xi^2) \] (24)

Note that the coefficients \( a_{1-3} \) and \( A_{1-3} \) depend on space and time through the macroscopic conserved variables, and so the second-order and mixed derivatives become

\[ \frac{\partial^2 f_0}{\partial t^2} = \frac{\partial A}{\partial t} f_0 + A \frac{\partial f_0}{\partial t} + a \frac{\partial^2 f_0}{\partial x^2} + \frac{\partial a}{\partial x} f_0 + a \frac{\partial f_0}{\partial x} \]
\[ \frac{\partial f_0}{\partial x \partial t} = \frac{\partial A}{\partial x} f_0 + A \frac{\partial f_0}{\partial x} \] (25)

Introducing the following definitions:

\[ B \equiv \frac{\partial A}{\partial t} \quad b \equiv \frac{\partial a}{\partial x} \quad C \equiv \frac{\partial A}{\partial x} \] (26)

it is possible to write the second and mixed derivatives the following relations:

\[ \frac{\partial^2 f_0}{\partial t^2} = (A^2 + B)f_0 \]
\[ \frac{\partial^2 f_0}{\partial x^2} = (a^2 + b)f_0 \]
\[ \frac{\partial^2 f_0}{\partial x \partial t} = (C + Aa)f_0 \] (27)

Substituting Eqs. (23,27) in Eq. (21) and in Eq. (22), the first and second nonequilibrium terms become

\[ Df_0 = (A + ua)f_0 \]
\[ D^2 f_0 = [(A^2 + B) + 2u(C + Aa) + u^2(a^2 + b)]f_0 \] (28)

Note that the functions \( b, B, \) and \( C \) have the same functional dependence on the collision invariants as the functions \( a \) and \( A \) in Eq. (24).

To compute the integrals of the nonequilibrium terms in the regularization formula for the collision time, the coefficients for the five functions \( a, b, A, B, \) and \( C \) in Eq. (28) have to be determined. To this end, the conservation constraint (i.e., the compatibility condition) allows the following:

\[ \int \psi Df_0 = 0 \quad \int \psi D^2 f_0 = 0 \] (29)

Substituting Eq. (28) into Eq. (29) results in the following:

\[ \int \psi [(A^2 + B) + 2u(C + Aa) + u^2(a^2 + b)]f_0 = 0 \] (30)

The conservation principle also states that

\[ \frac{\partial}{\partial x} \int \psi (\frac{\partial f_0}{\partial x}) = 0 \] (31)

which gives a third relation in the following form:

\[ \int \psi [(C + Aa) + v(a^2 + b)]f_0 = 0 \] (32)

Recalling now the microscopic definition of the macroscopic conserved quantities, it is possible to state two more relations for the spatial derivatives:

\[ \frac{dw}{dx} = \int \psi af_0 \quad \frac{d^2w}{dx^2} = \int \psi (a^2 + b)f_0 \] (33)

that close the balance unknowns/equations. Once the coefficients for \( a \) and \( b \) from Eq. (33) are computed, Eqs. (30,32) provide the coefficients for \( A, B, \) and \( C \) to compute the moments \( \langle Df_0 \rangle \) and \( \langle D^2 f_0 \rangle \) and finally the collision time from Eq. (18). The computation of both first- and the second-order derivatives of the macroscopic variables at the cell interface are here obtained by means of simple finite-difference formulas, i.e., referring to Fig. 4.

\[ \frac{dw}{dx} = \frac{w_{i+1} - w_i}{d_{ik}} \quad \frac{d^2w}{dx^2} = \frac{(w_{i+2} - w_{i+1})/d_{ik} + (w_i - w_{i-1})/d_{ik}}{d_{ik} + 0.5d_{i+1} + 0.5d_{i-1}} \]

The adoption of finite-difference formulas instead of the cubic reconstruction approach adopted initially by Xu [20] may introduce artificial numerical diffusion in the solution, but comparisons of the results obtained with the two approaches showed that no significant

![Fig. 4](image-url)
difference is observed, provided the flowfield and especially the shock waves are well resolved.

In the two-dimensional case, the procedure is almost the same, with the only difference being that now the distances $d_i$, $d_{i+1}$, and $d_{i+2}$, should be replaced with the relative projections along the relevant direction, and the functions $a$, $A$, $b$, $B$, and $C$ become

$$
    a(y) = a_1 + a_2 y + a_3 y^2 + a_4 \frac{1}{2} (y^2 + \xi^2), \\
    A(y) = A_1 + A_2 y + A_3 y^2 + A_4 \frac{1}{2} (y^2 + \xi^2), \ldots \\
    C(y) = C_1 + C_2 y + C_3 y^2 + C_4 \frac{1}{2} (y^2 + \xi^2).
$$

E. Identification of the Continuum Breakdown

Despite being introduced to account for the transitional regime, Eqs. (18,20) can be applied also in the case of the continuum regime. Nevertheless, the computational burden associated to this formulation makes this choice not very cost effective. To reduce the simulation time, a criterion to identify the local flow conditions at each node of the grid has been adopted that allows for automatically switching between the continuum formulation and the transitional one as the fluxes are computed. It is important to note that this technique is not used to decompose the domain into different regions as it is done in standard hybrid approaches, but it is only used at a nodal level to select the appropriate formulation for $\tau$.

Following the work of Wang and Boyd [11], a local Knudsen number can be adopted as an indicator for the switch in $\tau$ formulas. It is computed as

$$
    Kn_{loc} = \max[Kn_p, Kn_T, Kn_U]
$$

with the following definitions:

$$
    Kn_p = \lambda \frac{\nabla \rho}{\rho}, \quad Kn_T = \lambda \frac{\nabla T}{T}, \quad Kn_U = \lambda \frac{\nabla |U|}{|U|}
$$

where $\lambda$ is the local mean free path of the molecules. In the present node-pair formulation, the local gradient of the macroscopic quantities is replaced with the directional derivatives along the interface normal $\eta_{lk}$:

$$
    Kn_q = \lambda \frac{\nabla q \cdot \eta_{lk}}{q}, \quad q \in \{\rho, T, |U|\}
$$

The choice of the threshold value of $Kn_{loc}$ by which to switch from one description to the other depends on the problem at hand, but it usually ranges from 0.001 to 0.05. Eventually, a check is made to ensure that $Kn_{loc}$ is computed on the basis of a suitable macroscopic state at the boundary, $w^{\partial x}$, and its relative gradient, $\nabla w^{\partial x}$. The definitions of $w^{\partial x}$ and $\nabla w^{\partial x}$ in the case of inflow-outflow boundary are obtained by a classical characteristics approach, while in the case of a plane of symmetry the nullification of the gradient as well as of the normal component of the velocity provides a sufficient number of conditions to fix the boundary state [38]. The treatment of the solid wall boundary condition requires a more sophisticated approach that will be addressed next.

Following the work of Maxwell [42], the distribution function at the wall can be considered to be made of two parts: one describing the particles hitting the wall, $f_{inc}$, and one associated to the particles being reflected, $f_{ref}$:

$$
    f^0 = \begin{cases} 
        f_{inc}(u, x, t) & u \cdot n_{wall} > 0 \\
        f_{ref}(u' \rightarrow u, x, t) & u \cdot n_{wall} < 0
    \end{cases}
$$

The distribution function $f_{inc}$ can be computed from the state of the gas at node $i$ (i.e., $w_0^{\partial x} = u_i$ and $\nabla w_0^{\partial x} = \nabla u_i$), while $f_{ref}$, the so-called scattering kernel, is obtained on the basis of the type of interaction with the wall. A coefficient $\zeta$ can be introduced to describe the tendency of the gas to accommodate to the state of the wall. It can be expressed as follows [22]:

$$
    \zeta = \frac{\rho_{inc} \cdot \nabla \rho_{inc} - \rho_{ref} \cdot \nabla \rho_{ref}}{\rho_{inc} - \rho_{wall}}
$$

where $\rho(u, \xi)$ is any function of the molecular velocity and internal degrees of freedom. The coefficient $\zeta$ determines the fraction of the molecules being absorbed and re-emitted diffusely by the wall, and it can be used to rewrite the scattering kernel as

$$
    f_{ref}(u' \rightarrow u, x, t) = \zeta f_{wall} + \left(1 - \zeta\right) \cdot f_{inc}(u, x, t)
$$

The application of the kinetic definition for the fluxes [Eq. (11)] to the computation of the boundary term in Eq. (10) is now addressed. Following the same approach of the domain flux, the $\partial$ boundary term can be computed as follows:

$$
    \bar{J}_{\partial x} = \int u \rho f^0 \, du \, dz
$$

where $u$ is the component of the molecular velocity along the $x$ axis that, by definition, is normal to the boundary itself; and $f^0$ is the distribution function at the boundary. Different from the domain term, $f^0$ is not obtained from the solution of a Riemann problem but, according to the state of the gas near the boundary, a direct approximation in terms of Chapman–Enskog expansion is adopted. Once the state of the gas at the boundary is identified, the distribution function $f^0$ is computed on the basis of a suitable macroscopic state at the wall.

IV. Kinetic Boundary Conditions

All of the terms in Eq. (39) can be obtained from the system of equations obtained by substituting Eq. (39) in the equation for the conservation of mass, i.e.,

$$
    \left\{ \begin{array}{l}
        \frac{\rho_{inc} - \rho_{wall}}{\Delta t} = \frac{1}{2} \int_0^{\Delta t} \int_0^\infty u f_{inc} \\
        \frac{1}{\Delta t} \left( \frac{\rho_{inc} - \rho_{wall}}{\Delta t} \right) = 2(1 - \zeta) \rho_{inc}
    \end{array} \right.
$$

In the case of isothermal wall (i.e., $\zeta = 1$), $\theta_{wall}$ is imposed as a known boundary condition, and the unknowns appearing in Eq. (41) are $\rho_{ref}$, $\theta_{ref}$, and $\rho_{wall}$. In this case, the missing relation can be obtained by means of the mass conservation in case of full accommodation to the wall that provides an explicit formula for $\rho_{wall}$:

$$
    \rho_{wall} = \frac{2 \sqrt{\pi \theta_{wall}}}{\Delta t} \int_0^{\Delta t} \int_0^\infty u f_{inc}
$$
In the case of the adiabatic wall (i.e., $\zeta = 0$), the distribution function at the wall is taken to be equal to $f_{\text{inc}}$; see Eq. (38). The application of the kinetic wall boundary condition [Eq. (38)] produces a boundary distribution function $f'_{\partial}$ for which the macroscopic velocity at the wall surface is zero only for very small values of the Knudsen number, allowing for a natural representation of the velocity and temperature slip effects.

The flow of air around a cylinder at $Ma_{\infty} = 4$ and for three different Knudsen numbers (i.e., $Kn_{\infty} = 0.01$, 0.1, and 0.3) is considered here to illustrate behaviour of the present boundary condition formulation. Air has a specific heat ratio $\gamma = 1.4$ and a Prandtl number $Pr = 0.72$. A Sutherland viscosity model has been adopted with the following values: $\mu_0 = 1.78 \times 10^{-5}$ Pa · s and $T_0 = 273$ K. The cylinder surface is isothermal with $T_{\text{wall}} = 288$ K. A hybrid mesh has been adopted for each simulation, and the solution procedure has been coupled with a recent mesh-adaptation procedure [44]. The size of the final adapted meshes for each case is summarized in Table 1. Figures 5 and 6 illustrate the slip velocity at cylinder’s wall for $Kn_{\infty} = 0.01$ and $Kn_{\infty} = 0.3$, respectively. The velocity profiles computed by the present node-pair–BGK scheme are compared with the solutions obtained by the classical macroscopic slip model by Gokcen and MacCormack [5]. The continuum breakdown is identified according to Eq. (34) with a threshold value of $Kn_{CB} = 0.05$, and the nonequilibrium regions are also presented in the same figures. These are the areas where the modified formula for the mean collision time is applied. Eventually, Fig. 7 shows the computation of the drag coefficient of the cylinder at the different

<table>
<thead>
<tr>
<th>$Kn$</th>
<th>Nodes</th>
<th>Triangles</th>
<th>Quadrilateres</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>154,843</td>
<td>97,787</td>
<td>105,551</td>
</tr>
<tr>
<td>0.1</td>
<td>159,196</td>
<td>117,973</td>
<td>99,804</td>
</tr>
<tr>
<td>0.3</td>
<td>159,642</td>
<td>126,379</td>
<td>96,039</td>
</tr>
</tbody>
</table>

![Fig. 5](source) Flow of air at Mach 4 and Kn 0.01. Identification of continuum-breakdown (left) and slip velocity (right).

![Fig. 6](source) Flow of air at Mach 4 and Kn 0.3. Identification of continuum-breakdown (left) and slip velocity (right).

![Fig. 7](source) Drag coefficient for air flow at Mach 4 and different Knudsen values.
Knudsen numbers and the comparison with experimental data available in the literature [9,45]. The match with the experimental data reduces as the Knudsen number increases due to the limitations of the present approach in modeling the gas–surface interaction as the rarefaction level increases.

V. Numerical Examples

The flow around a cylinder is characterized by features typical of the actual flow around space vehicles, such as the presence of a detached normal shock wave near a round-shaped nose or leading edge, together with the presence of a highly expanding flow in the rear part of the body. It has therefore been selected as a significant test case to explore local features typical of the aerospace missions. In this section, simulations of monoatomic and diatomic gases are considered. Tables 2 and 3 summarize the gas properties including Sutherland law parameters and the flow conditions for which the simulations have been performed. For completeness, the data for the simulations presented in the previous section are also included.

A. Argon Gas Flow at Mach 5.48

In the present section, three distinct numerical tests will be presented corresponding to values of the asymptotic Knudsen number that range from continuum to transitional regime, namely $Kn = 0.001$, $Kn = 0.025$, and $Kn = 0.3$ for the same speed ratio $S = u_{∞}/\sqrt{2RT_{∞}} = 5$. In these examples, the atmosphere is assumed to be made by argon, a monatomic gas having a specific heat ratio $\gamma = 5/3$ and Prandtl number $Pr = 0.667$. The Sutherland viscosity model has been considered with the following characteristic values: $\mu_0 = 2.515 \times 10^{-5}$ Pa · s and $T_0 = 273$ K. The asymptotic Mach number is $Ma_∞ = 5.48$, and the cylinder temperature is $T_{wall} = 273.15 \text{K}$. A relation exists between the mean free path of the molecules $\lambda$ and the dynamic viscosity of the argon (i.e., $\mu = 5\sqrt{2\pi R T_{wall}}/16$) by which it is possible to obtain a formula that links together the asymptotic Mach ($Ma_∞$), Knudsen ($Kn_∞$), and Reynolds ($Re_∞$) numbers [20,46]:

$$Re_∞ = \frac{16}{5} \sqrt{\frac{\gamma Ma_∞}{\pi Kn_∞}}$$

By virtue of Eq. (43), it is possible to obtain the Reynolds numbers associated to the three flow conditions, summarized in Table 4. The considered flows can safely be assumed to be laminar.

A hybrid grid made of both triangles and quadrilateral elements has been adopted for the present simulations, and the whole solution procedure has been paired with a procedure for the automatic adaptation of the mesh [44]. In all cases, the initial size of the grid is 4116 nodes and 6105 elements.

The first results presented are for $Kn = 0.001$, which is a continuumlike flow. The mesh that guarantees grid independence is obtained after five adaptation levels, and it is made of 165,260 nodes and 241,193 elements (87,940 triangles and 153,253 quadrilaterals). Figure 8 shows temperature and Mach number contours. The shock is very sharp, and the downstream region is characterized by a well-defined laminar wake. Figure 9 shows the comparison of the density and velocity profiles along the stagnation line with the solution obtained with a finite-volume code, based on a classical macroscopic formulation of the Navier–Stokes fluxes. As can be observed, the solution obtained by the standard macroscopic scheme and the present node-pair–BGK are almost superimposed, and no visible difference is revealed.

The results of the computations for $Kn = 0.025$ and $Kn = 0.3$, for which the transitional regime is established, are based on adapted meshes that are made of 145,606 nodes and 239,532 elements (145,606 nodes and 239,532 elements) for the flow at $Kn = 0.025$ and 104,045 nodes and 192,271 elements (153,253 quadrilaterals) for $Kn = 0.3$. The node-pair–BGK results have been compared to the direct simulation Monte Carlo (DSMC) results of Vogenitz et al. [47] and to the results of Yang and Huang [46]. The latter adopted a numerical scheme based on the discrete ordinates method to solve the Boltzmann equation, in which a reduced distribution function approximation has been considered together with a discretization of the distribution function in the space of the molecular velocities [46]. Figures 10 and 11 show the results for the

---

**Table 2** Gas properties and Sutherland law parameters

<table>
<thead>
<tr>
<th>$C_p/C_v$</th>
<th>Prandtl</th>
<th>$\mu_0$, Pa/s</th>
<th>$T_0$, K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>1.4</td>
<td>0.72</td>
<td>1.78 $\times 10^{-5}$</td>
</tr>
<tr>
<td>Ar</td>
<td>1.667</td>
<td>0.67</td>
<td>2.515 $\times 10^{-5}$</td>
</tr>
<tr>
<td>$N_2$</td>
<td>1.4</td>
<td>0.72</td>
<td>1.661 $\times 10^{-5}$</td>
</tr>
</tbody>
</table>

**Table 3** Flow conditions

<table>
<thead>
<tr>
<th>Mach</th>
<th>Kn</th>
<th>Re</th>
<th>$T_{wall}$, K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>4.0</td>
<td>0.01</td>
<td>604.2</td>
</tr>
<tr>
<td>Air</td>
<td>4.0</td>
<td>0.1</td>
<td>60.4</td>
</tr>
<tr>
<td>Air</td>
<td>4.0</td>
<td>0.3</td>
<td>20.1</td>
</tr>
<tr>
<td>Ar</td>
<td>5.48</td>
<td>0.001</td>
<td>9031.61</td>
</tr>
<tr>
<td>Ar</td>
<td>5.48</td>
<td>0.025</td>
<td>361.26</td>
</tr>
<tr>
<td>Ar</td>
<td>5.48</td>
<td>0.3</td>
<td>30.105</td>
</tr>
<tr>
<td>$N_2$</td>
<td></td>
<td>0.0118</td>
<td>1564.43</td>
</tr>
</tbody>
</table>

**Table 4** Knudsen and Reynolds numbers

<table>
<thead>
<tr>
<th>Kn</th>
<th>Re</th>
<th>Regime</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>9031</td>
<td>Continuum</td>
</tr>
<tr>
<td>0.025</td>
<td>361</td>
<td>Transitional</td>
</tr>
<tr>
<td>0.3</td>
<td>30</td>
<td>Transitional</td>
</tr>
</tbody>
</table>

---

**Fig. 8** Continuum-like flow of argon at Ma 5.48 and Kn 0.001. Temperature contours (left) and Mach number (right).
Fig. 9  Stagnation line profiles for the cylinder at Ma 5.48 and Kn 0.001. Normalized density (left) and normalized velocity (right).

Fig. 10  Transitional flow of argon at Ma 5.48 and Kn 0.025. Temperature contours (left) and Mach number (right).

Fig. 11  Stagnation line profiles for the cylinder at Ma 5.48 and Kn 0.025. Normalized density (left) and normalized velocity (right).

Fig. 12  Hypersonic transitional flow of Argon at Ma 5.48 and Kn 0.3. Temperature contours (left) and Mach number (right).
case at Kn = 0.025 while Figs. 12 and 13 show the results for the case at Kn = 0.3. It is well evident from the Mach plots how the shock thickness increases with Kn and the downstream wake gradually disappears. Figures 11 and 13 show the distribution of the normalized density and velocity along the stagnation line and the agreement with DSMC is satisfactory. Less diffusion is observed with respect to the discrete ordinate method by Yang and Huang [46] even though a slight discrepancy in the density profile is observed in the postshock region at Kn = 0.3. Figures 14 and 15 are eventually included to show the inaccuracy of standard macroscopic Navier–Stokes schemes in the transitional regime. These show the comparison of the results obtained with the present BGK method, the DSMC particle method, and a Navier–Stokes solver in terms of velocity and temperature profiles along the stagnation line.

Fig. 13  Stagnation line profiles for the cylinder at Ma 5.48 and Kn 0.3. Normalized density (left) and normalized velocity (right).

Fig. 14  Comparison of the velocity profiles with macroscopic Navier–Stokes approach: Kn 0.025 (left) and Kn 0.3 (right).

Fig. 15  Comparison of the temperature profiles with macroscopic Navier–Stokes approach: Kn 0.025 (left) and Kn 0.3 (right).
flows that range from the continuum up to the transitional regime in a unified manner. The contribution of the present work consists of the kinetic-Bhatnagar–Gross–Krook reformulation of the node-pair discretization of conservation laws. This methodology allows for a unified treatment of different flow regimes, up to the transitional one, together with the high flexibility to work with unstructured grids made of mixed elements. As a consequence, the present node-pair formulation allows simulation, efficiently and on a genuine multidimensional basis, of problems typical of many aerospace missions, where both geometrical complexity and coexistence of different equilibrium conditions exist.

Exemplary test cases have been selected to analyze the performances of the proposed method. The results show fair agreement with standard macroscopic-based solvers for the continuum part and with particle-based methods and other kinetic approaches for the transitional part. Improvement in the quality of the present results is expected from the inclusion of more detailed models of the flow physics. Currently, separate modeling for the rotational and vibrational temperatures as well as the inclusion of chemical reaction effects are not available. This is not, however, a limitation intrinsic to the proposed approach, which can be extended to a multiple-distribution formulation to account for more-sophisticated nonequilibrium flows.

An analysis of how far it is possible to go into the rarefied regime with the present approach has not been performed yet. Nevertheless, it has to be observed that, because the current implementations and computational resources allow standard particle-based methods like direct simulation Monte Carlo to simulate ranges of Knudsen number of the order of $10^{-1}$ at a reasonable computational expense, the former analysis will have more an academic flavor rather than a practical outcome in the modeling and simulation of hypersonic rarefied flows. The extension of the approach to a three-dimensional formulation is currently under development.

### VI. Conclusions

The present paper addresses the formulation and implementation of a node-pair-based kinetic scheme for the numerical simulation of


X. Zhong
Associate Editor