Rapid Communications

Gas-kinetic simulation of sustained turbulence in minimal Couette flow

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We provide a demonstration that gas-kinetic methods incorporating molecular chaos can simulate the sustained turbulence that occurs in wall-bounded turbulent shear flows. The direct simulation Monte Carlo method, a gas-kinetic molecular method that enforces molecular chaos for gas-molecule collisions, is used to simulate the minimal Couette flow at $\mathrm{Re} = 500$. The resulting law of the wall, the average wall shear stress, the average kinetic energy, and the continually regenerating coherent structures all agree closely with corresponding results from direct numerical simulation of the Navier-Stokes equations. These results indicate that molecular chaos for collisions in gas-kinetic methods does not prevent development of molecular-scale long-range correlations required to form hydrodynamic-scale turbulent coherent structures.

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Turbulent flows are characterized by coherent structures [1], which are long-range correlations that survive over long times and distances [2]. These coherent structures grow out of "noise" and interact with each other and nearby walls, thereby sustaining turbulence through a continual cycle of regeneration and decay while simultaneously enabling energy to cascade from larger to smaller scales. Formation of coherent structures at the hydrodynamic scale requires long-range correlations at the molecular scale over distances significantly longer than the gas-molecule mean free path. Unlike steady laminar flow, in which correlations are merely preserved, sustained turbulent flow has correlations that continually form, propagate, decay, and regenerate.

The question of whether gas-kinetic methods that employ molecular chaos, which include the Boltzmann equation (BE), are capable of simulating sustained turbulent flow in a gas was first posed a half century ago by multiple investigators [3–12]. Although gases are usually simulated using continuum hydrodynamic methods, gas-kinetic molecular methods are often used when thermal fluctuations, thermodynamic nonequilibrium, rarefaction, or chemical reactions are important [13]. Deterministic molecular-dynamics (MD) methods [14], which treat N-body interactions accurately and thus inherently maintain correlations, could also be used in principle, but they have high computational costs compared to gas-kinetic methods. However, whether molecular chaos would allow or prevent gas-kinetic methods from forming the long-range correlations required to form the coherent structures that sustain turbulent flow remained unclear.

Answering this question generated some controversy because of the ambiguity of the role of the assumption of molecular chaos in the derivation of the BE. More specifically, some investigators explicitly use this assumption, but other investigators use different assumptions that are not obviously equivalent to assuming molecular chaos. Moreover, part of this controversy revolves around precisely

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what is meant by the assumption of molecular chaos. Heuristically, molecular chaos implies a lack of correlation between molecular quantities in space and/or time [5], but how this lack of correlation is applied differs from one investigator to another.

Some investigators [3,4,9–12] applied the idea of molecular chaos in a broad sense. More specifically, they enforced this lack of correlation globally throughout the gas. In this approach, all correlations present in the initial state are ignored. This interpretation of molecular chaos appears to preclude the development of turbulent flow because molecules fail to retain the long-range correlations essential for sustained turbulent flow. With this rationale, Tsugé [10] asserted that molecular chaos prevents gas-kinetic methods such as the BE from forming long-range correlations and thus questioned the ability of gas-kinetic methods to simulate sustained turbulent flow. By truncating the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) [3,4] hierarchy to two points without assuming molecular chaos, Grad, Tsugé, and Sastri derived a generalized BE and showed that this equation allows long-range correlations. They subsequently derived the Navier-Stokes equations (NSEs) from low-order moments of their generalized BE, so they inferred that molecular chaos must be absent from gas-kinetic methods in order for such methods to allow correlations and thereby simulate sustained turbulent flow.

Other investigators [5–7] applied the idea of molecular chaos in a more restricted sense. More specifically, they enforced molecular chaos for gas-molecule collisions but not for gas-molecule motion between collisions. Thus, gas molecules lose correlation only during collisions but retain correlation in space and time during motion from one location to another (transport). This approach is motivated by the fact that the gas-molecule mean free path is typically much longer than the range of the forces that govern gas-molecule collisions [5]. With this more limited assumption, Kogan [6] achieved the same truncation of the BBGKY hierarchy and derived the BE. In contradistinction to Grad, Tsugé, and Sastri, Kogan thus suggests that enforcing molecular chaos only for gas-molecule collisions does not prevent the formation of coherent structures necessary for sustained turbulent flow because molecules retain spatial and temporal correlation as they move from one location to another [6].

Hence, the ability of gas-kinetic methods to allow the formation, propagation, decay, and regeneration of the long-range correlations necessary for establishing the coherent structures essential for sustaining turbulence has been debated but has never been formally proved or unambiguously demonstrated. This statement applies not only to gas-kinetic methods like the BE, which directly solves for the molecular velocity distribution, but also to gas-kinetic molecular methods like Bird's direct simulation Monte Carlo (DSMC) method [15], which indirectly solves for the molecular velocity distribution by tracking large numbers of computational molecules that move and collide. Gallis *et al.* [16–18] did show that DSMC can accurately simulate flow instabilities and decaying homogeneous isotropic turbulence. However, they did not show that DSMC can simulate sustained turbulence (which requires continual regeneration of long-range correlations and the associated coherent structures), as opposed to decaying turbulence (which does not require such regeneration). Thus, the question addressed here is whether gas-kinetic methods like the BE and DSMC, which enforce molecular chaos only for collisions, allow the long-range correlations associated with the coherent structures that sustain turbulent flow.

DSMC [15] is a gas-kinetic molecular method that has been proved to yield solutions to the BE in the limit of vanishing numerical error [19–21]. Like the BE, DSMC is appropriate when the gas-molecule mean free path is much larger than the gas-molecule diameter (usually the case). DSMC uses a stochastic algorithm that approximates the velocity distribution function with a discrete number of computational molecules or "particles." Each particle typically represents a large number of real molecules, and these particles move, collide with other particles, and reflect from boundaries just as real molecules do.

To ascertain whether gas-kinetic methods enforcing molecular chaos for collisions only can simulate sustained turbulence in wall-bounded shear flows, DSMC simulations are performed of the minimal Couette flow (MCF). The point is not to demonstrate that molecular methods can simulate turbulence: MD simulations of the MCF for liquids have already been performed [22]. Nor

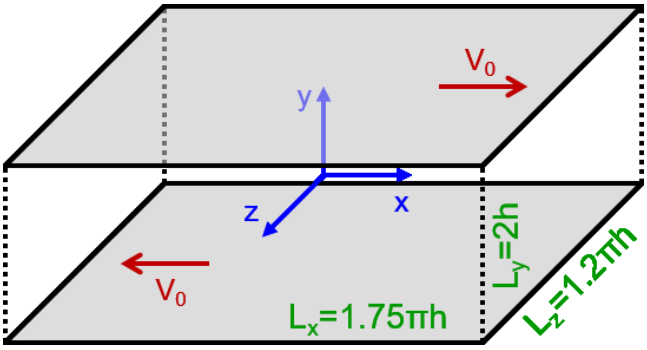

FIG. 1. MCF physical domain.

is the point to glean new physical insights into this flow: the MCF has been used extensively to study the process by which the coherent structures sustaining turbulence form, propagate, decay, and regenerate [23–25]. Instead, the MCF is investigated here precisely because it is a generic wall-bounded turbulent shear flow in which the regeneration process has been well characterized.

The MCF is a geometrically constrained three-dimensional Couette flow (see Fig. 1). The domain is a rectangular cuboid bounded by walls on two opposite sides, and the origin of the coordinate system is located at the center of the cuboid. Its length in the x direction (streamwise) is $L_x = 1.75\pi h$, its length in the z direction (spanwise) is $L_z = 1.2\pi h$, and the corresponding pairs of boundaries are periodic. The walls are separated in the y direction (normal) by a distance $L_y = 2h$ and slide in the x direction with tangential velocities $u_w = \pm V_0$. Typically, the no-slip boundary condition is applied on the walls so that $u = \pm V_0$ at $y = \pm h$, respectively. In the DSMC simulations, these walls are fully accommodating. A fully accommodating wall reflects the incident particles so that the reflected particles have a velocity distribution function in equilibrium with the wall velocity and temperature [15]. This boundary condition enforces impermeability but allows a nonzero slip velocity to exist between the wall and the gas in the presence of shear. When the mean free path λ is small relative to the gap half-height h (as is the case in these simulations), this slip velocity u_s is small compared to the wall velocity $u_w = V_0$. The normalized time is defined as $T = V_0 t/h$, and the Reynolds number is defined as $\mathrm{Re} = V_0 h/\nu$, where $\nu = \mu/\rho$ is the kinematic viscosity for a gas of density ρ and dynamic viscosity μ.

DSMC simulations of the MCF are performed at $\mathrm{Re} = 500$. This value is used because results from direct numerical simulation (DNS) of the NSEs indicate that turbulence is not sustained below $\mathrm{Re} \approx 300$ [23]. The gap half-height is $h = 500\mu$m, and the domain is divided into $1982 \times 721 \times 1359$ cells (about 2 billion in total), which yields nearly cubical cells with a side length of $\Delta s = 1.387\mu$m. Each of these cells has an average of 30 particles per cell (about 58 billion particles in total). To improve the spatial discretization, collision partners in a cell are selected from other particles lying within a sphere having a radius that equals the distance traveled by the particle during a time step. The gas has the molecular mass and specific heat ratio of argon ($m = 66.3 \times 10^{-27}$ kg, $\gamma = 5/3$ [15]) and an initial pressure and temperature of $p_0 = 18\,190$ Pa and $\theta_0 = \theta_w = 273.15$ K (the wall value), which corresponds to a sound speed of $c_0 = 307.9$ m/s. The wall velocity is $V_0 = 92.35$ m/s, which corresponds to a Mach number of 0.3, so the simulation conditions marginally satisfy the incompressibility assumption [26]. A time step of $\Delta t = 45.6$ ps is used, so particles move roughly 1% of the cell size during each time step.

Initially, the gas has a velocity field that is the sum of laminar Couette flow ($u = V_0 y/h$) plus a perturbation. A perturbation is needed to enable the MCF to become turbulent because linear stability theory indicates that laminar Couette flow is stable for all Reynolds numbers [23]. DSMC simulations initialized with only the unperturbed laminar profile remain laminar until the simulations terminate (at $T = 100$), in agreement with linear stability theory.

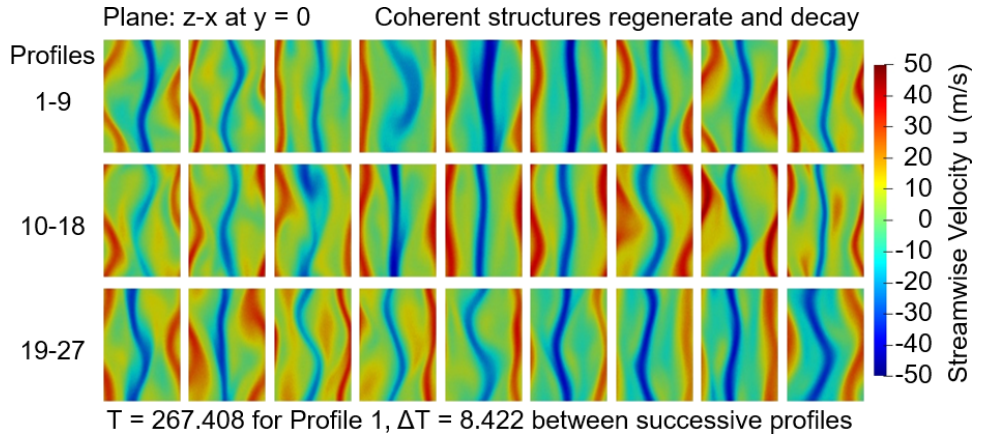

FIG. 2. DSMC MCF streamwise velocity profiles on midplane between walls show sustained turbulence with several cycles of regeneration and decay of coherent structures.

Gas-molecule collisions are performed using the hard-sphere (HS) collision model [15], which produces a viscosity proportional to the square root of the temperature. The discretization errors in DSMC act to increase the effective transport properties [27]. For these simulations, the effective viscosity μ and hence the effective Reynolds number Re are determined by comparing a one-dimensional DSMC simulation of laminar Couette flow (the domain consists of a single column of three-dimensional cells in the y direction) to the analytical expression for the wall shear stress of laminar Couette flow ($\tau = \mu V_0/h$). This comparison indicates that the discretization used for these simulations leads to an effective Reynolds number of $\mathrm{Re} = 500$.

The DSMC code SPARTA [28,29] is used to perform these simulations. SPARTA is an exascale-class open-source code capable of running efficiently on massively parallel, heterogeneous-architecture computational platforms. The MCF simulations are performed on Sequoia, an IBM Blue Gene/Q supercomputer, and use just over a million MPI tasks on a half-million cores (32 K nodes, 1/3 of the machine) for 1200 hours.

To assess the DSMC simulations, corresponding DNS simulations are performed using the spectral element code NEK5000 [30]. The fluid is continuum, incompressible, and isothermal. The DNS domain is discretized using 32 seventh-order spectral elements along each coordinate direction, with each element containing 8^3 grid points at the Gauss-Lobatto nodes, for a total of 256 grid points along each side of the domain. To confirm mesh independence, the simulations are repeated with 192 and 320 grid points along each coordinate axis, with no significant changes observed in the turbulence statistics (e.g., Reynolds stresses change by less than 2%). The DNS simulations are initialized with the same initial conditions used in the DSMC simulations. To ensure sampling statistics from a fully turbulent flow field, the DNS simulation is run without sampling until $T = 200$ and then run with sampling up to $T = 3000$. Convergence of the turbulence statistics is quantified by monitoring the profile of average shear stress through the channel, which is constant for statistically converged turbulent Couette flow. Here, the average shear stress profile differs from a constant by less than 0.6% across the channel, indicating sufficient sampling.

Figure 2 presents DSMC profiles of the streamwise velocity component u on the midplane between the walls ($y = 0$) at 27 consecutive times for the MCF. The first profile is at time $T = 267.408$, and adjacent profiles are separated by a time increment of $\Delta T = 8.422$. Two vortices of opposite sense that are oriented predominantly in the streamwise direction are present. These vortices have diameters comparable to the gap height $2h$, so two vortices fit well into the spanwise extent of the domain since $L_z \approx 2L_y$. As time progresses, these vortices pass through several cycles of regeneration and decay: the vortices are disrupted significantly in profiles 4, 8, 12, 16, and 20, and more vortices appear

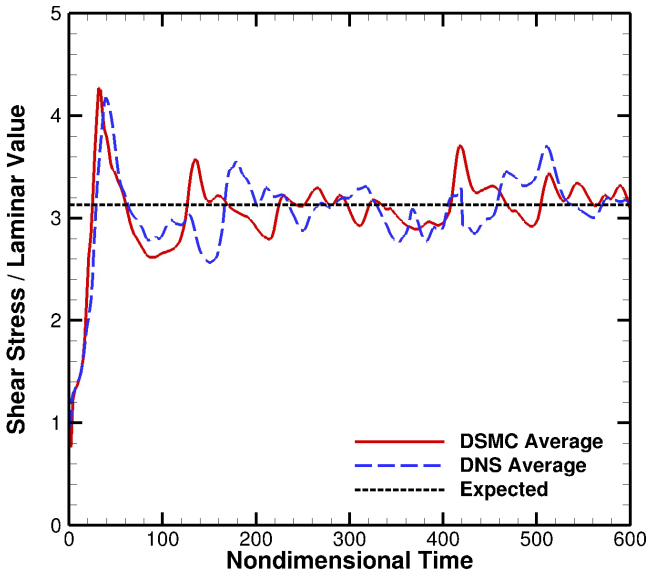

FIG. 3. Shear stress averaged over both walls versus time from DSMC and DNS simulations.

transiently in profiles 18, 21, 22, and 26. This continuous cycle of regeneration and decay sustains the turbulence in this flow. As discussed earlier, the details of the kinematics and dynamics of regeneration and decay have been discussed extensively in the literature [23–25] and are not the subject of this work.

Figure 3 presents the shear stress from DSMC and DNS averaged over both walls as functions of time, and Fig. 4 presents the volume-averaged kinetic energy from both methods. Here, the turbulent values are normalized by their laminar values: $\tau_{\text{lam}} = \mu V_0/h$, $k_{\text{lam}} = \rho V_0^2/6$. Over the time interval of $T = 200-600$, the DSMC simulation yields a normalized shear stress of 3.13 ± 0.18, which

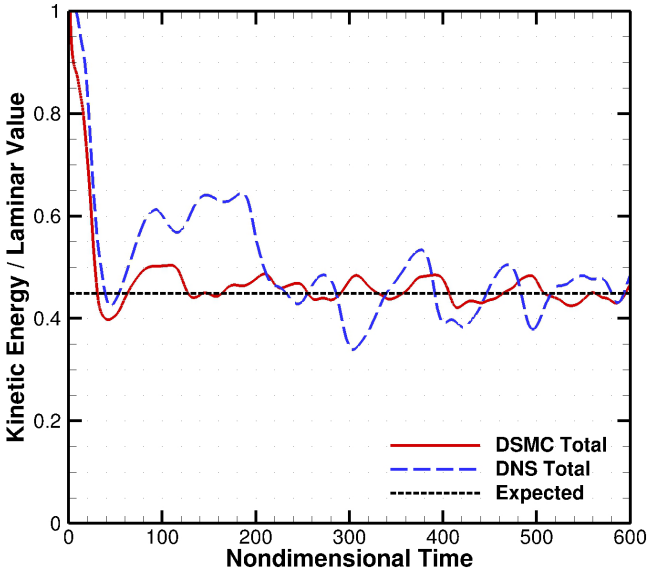

FIG. 4. Average kinetic energy per unit volume versus time from DSMC and DNS simulations.

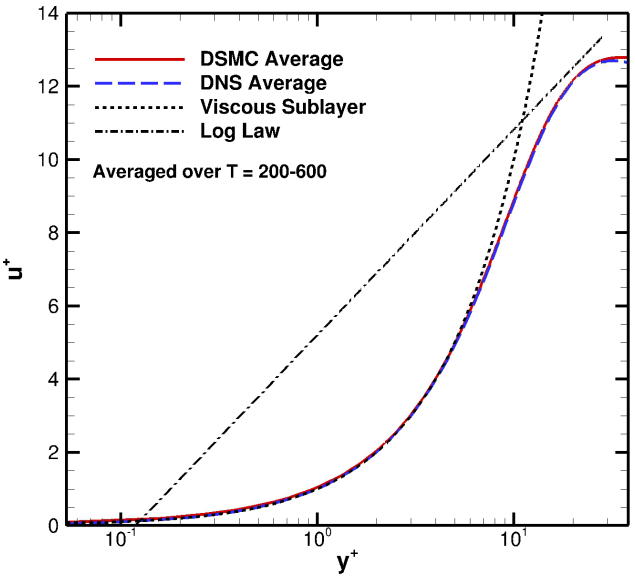

FIG. 5. Law of the wall from DSMC and DNS simulations.

agrees closely with the corresponding DNS value of 3.13 ± 0.20 (if the DNS averaging duration is increased to $T = 200-3000$, the expected value is unchanged). Similarly, the DSMC simulation yields a normalized kinetic energy of 0.449 ± 0.048, which again agrees closely with the DNS value of 0.449 ± 0.047. Although not identical in detail because turbulent flow is chaotic, the DSMC and DNS fluctuations have similar magnitudes and durations.

The quasiperiodic random fluctuations observed in the shear stress and the kinetic energy are an essential feature of turbulent flow and are characteristic of the regeneration and decay process [23]. These fluctuations indicate that the long-range correlations leading to these coherent structures continually regenerate and decay in the DSMC simulation. Thus, the agreement between the DSMC and DNS results suggests that DSMC, a gas-kinetic molecular method that enforces molecular chaos only in collisions, does continually regenerate the long-range correlations and coherent structures necessary to sustain turbulence in wall-bounded shear flows. This conclusion goes beyond those of Grad [9], Tsugé [10], Sastri [11], and Tsugé and Sagara [12].

Figure 5 presents the mean velocity profiles from the DSMC and DNS simulations. These profiles are found by averaging the streamwise velocity component u over times of $T = 200-600$ and over the streamwise and spanwise coordinates x and z at each fixed value of the normal coordinate y. The resulting profiles are plotted using standard wall-based quantities: position $y^+ = \hat{y}v^*/\nu$ and velocity $u^+ = \hat{u}/v^*$, where $v^* = \sqrt{\tau_w/\rho}$, $\hat{y} = |y_w - y|$, $\hat{u} = |u_w - u|$, $y_w = \pm h$, $u_w = \pm V_0$, and τ_w is the average wall shear stress. The profiles from both walls are virtually indistinguishable, so their average is presented. The DSMC and DNS mean velocity profiles are almost identical and agree closely with the inner law $u^+ = y^+$ in the viscous sublayer ($y^+ < 8$). The log law $u^+ = (1/\kappa)\ln y^+ + B$ with $\kappa = 0.41$ and $B = 5.1$ is plotted for comparison. The DSMC and DNS mean velocity profiles approach the log law from below near $y^+ = 20$, but the Reynolds number of $\mathrm{Re} = 500$ is too low for the log law to be observed over a large portion of the domain. Although the DNS profiles exactly satisfy the no-slip condition at the walls, the DSMC profiles have a slip velocity of $u_s \approx 0.5\,\mathrm{m/s}$, which is small relative to the wall velocity of $V_0 = 92.35\,\mathrm{m/s}$ and thus not dynamically significant.

The many aspects of agreement between the DSMC and DNS results indicate that the nonlinear regeneration processes in gas-kinetic methods (e.g., the BE) and continuum methods (e.g., the NSEs) are basically the same. The fact that the DSMC and DNS results agree closely for the MCF, a canonical wall-bounded turbulent shear flow, indicates that gas-kinetic methods like DSMC and,

by extension, the BE that enforce molecular chaos for gas-molecule collisions can be used for quantitative investigations of turbulence. This conclusion is of significance to gas-kinetic theory because the assumption of molecular chaos for gas-molecule collisions plays key roles in derivations of the BE and of gas-kinetic molecular methods like DSMC. Conversely, DSMC could complement DNS because phenomena such as thermal relaxation and chemical reactions can be incorporated into DSMC at the molecular level in a straightforward manner.

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