

**Steady Periodic Shear Flow *is* Stable in Two Space Dimensions .
Nonequilibrium Molecular Dynamics *versus* Navier-Stokes-Fourier
Stability Theory – A Comment on two Arxiv Contributions .**

Wm. G. Hoover and Carol G. Hoover

Ruby Valley Research Institute

Highway Contract 60, Box 601

Ruby Valley, Nevada 89833

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Abstract

Dufty, Lee, Lutsko, Montanero, and Santos have carried out stability analyses of steady stationary shear flows. Their approach is based on the compressible and heat conducting Navier-Stokes-Fourier model. It predicts the unstable exponential growth of long-wavelength transverse perturbations for both two- and three-dimensional fluids. We point out that the patently-stable two-dimensional periodic shear flows studied earlier by Petravic, Posch, and ourselves contradict these predicted instabilities. The stable steady-state shear flows are based on *nonequilibrium* molecular dynamics with simple *thermostats* maintaining nonequilibrium stationary states in two space dimensions. The failure of the stability analyses remains unexplained.

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I. INTRODUCTION

It recently came to our attention that the *stability* of high-Reynolds'-number atomistic shear flows¹⁻⁵ apparently contradicts the *instability* predicted by a perturbation analysis^{6,7} of the Navier-Stokes-Fourier equations for steady compressible heat-conducting simple shear. Here we develop an algorithm for solving the Navier-Stokes-Fourier problem directly. We also apply a two-dimensional version of the perturbation analysis to soft disks. This work confirms the contradictory nature of the microscopic and macroscopic approaches. The failure of the perturbation analysis remains unexplained.

In Section II we describe the atomistic and continuum approaches to simulating simple shear. We apply the continuum algorithm^{8,9} to a Navier-Stokes-Fourier gas-phase model of simple shear. In Section III we formulate a dense-fluid constitutive model^{3,10,11} for the *continuum* description of the soft disks used in *atomistic* simulations. In Section IV we apply several versions of the continuum perturbation theory to this soft-disk constitutive model. The results of that theory are contradicted by the existing molecular dynamics results. Section V sums up the current state of our knowledge, emphasizing the open problem which remains unsolved.

II. STEADY SHEAR FLOWS IN TWO SPACE DIMENSIONS

Steady homogeneous shear flows with periodic boundaries would seem to be the simplest conceivable nonequilibrium steady states. Figure 1 shows a particle snapshot taken from a typical molecular dynamics simulation. In that Figure the central cell, containing $N = 100$ two-dimensional particles, is repeated periodically in space. Periodic images to the right and to the left are generated by adding or subtracting multiples of the cell side length L to all the particle coordinate values from the central cell. 100-particle images just above the central cell move to the right with an additional velocity $+\dot{\epsilon}L$ relative to the central row of cells. Images just below that row likewise move to the left with an additional velocity $-\dot{\epsilon}L$. These periodic boundaries impose a shear strain rate and a corresponding stress on *all* cells. The *strain rate* $\dot{\epsilon}$ defined and imposed by these periodic boundary conditions is the overall macroscopic velocity gradient :

$$\dot{\epsilon} \equiv \langle du_x/dy \rangle .$$

N = 100, Periodic Shear Flow

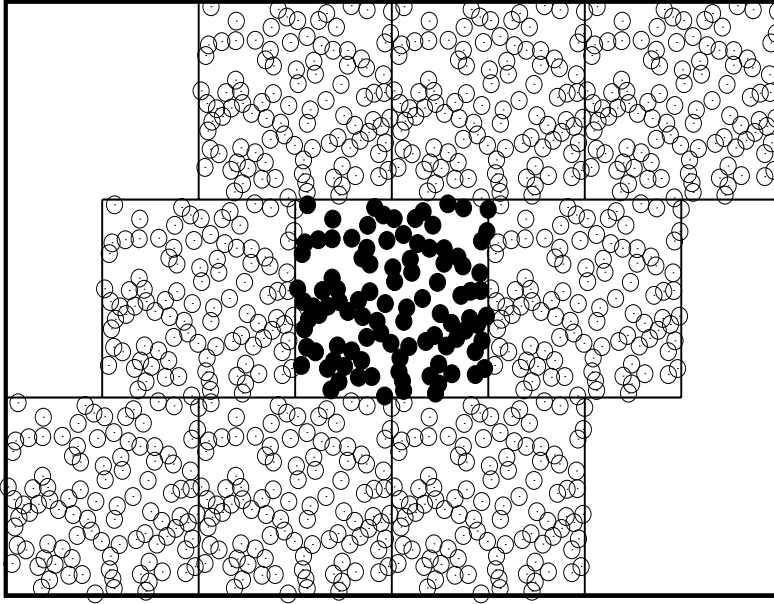


Figure 1: Snapshot from a molecular dynamics simulation of steady periodic shear in two space dimensions. The three periodic images of the central $L \times L$ cell shown in the top row move to the right with velocity $+\dot{\epsilon}L$ relative to the central 100-particle cell. The three images in the bottom row move to the left with velocity $-\dot{\epsilon}L$. The regular checkerboard arrangement of the cells recurs at integral multiples of the shear period, $\tau = (1/\dot{\epsilon})$.

Such early 100-particle studies from the 1970s were, by the 1990s, augmented by larger-scale simulations with as many as $514^2 = 264,196$ particles¹⁻⁵. These *steady-state* flows, in which the heat generated by the shearing motion is extracted by “thermostat” (or ergostat) forces, established that the measured shear viscosity, at fixed strain rate, is insensitive to system size.

Consider a prototypical dense soft-disk fluid, with $N = L^2$ and a short-ranged repulsive pair interaction $\phi(r < 1) = 100(1 - r^2)^4$. For N greater than 64 the shear viscosity has only a small “size dependence”. For a fixed strain rate the finite- N viscosity $\eta(\dot{\epsilon}, N)$ approaches the large-system limit from below. The N -dependent deviations from the limiting viscosity, $\eta(\dot{\epsilon}, N \rightarrow \infty)$, are of order $\sqrt{(1/N)}$. The deviation is about two percent for $N = 64$ and is negligible, relative to statistical fluctuations, for systems with N of order 10,000^{3,4}.

One might well expect, by analogy with macroscopic three-dimensional hydrodynamic flows¹², that a *turbulent* instability would appear at a Reynolds’ Number of the order of a thousand, $R \equiv \dot{\epsilon}L^2/(\eta/\rho) \simeq 1000$. In fact, detailed investigations, for thermostated two-

dimensional flows with Reynolds' Numbers as large as 50,000 , showed *no instability whatever*. These molecular dynamics simulations showed instead that steady two-dimensional dense-fluid shear flows are stable. These results were announced in 1995 in two papers by author Bill and Harald Posch, “Large-System Hydrodynamic Limit” and “Shear Viscosity *via* Global Control of Spatiotemporal Chaos in Two-Dimensional Isoenergetic Dense Fluids”.

Soon afterward two papers suggesting a long-wavelength exponential *instability of all* such flows appeared in the Condensed Matter arXiv: “Stability of Uniform Shear Flow” and “Long Wavelength Instability for Uniform Shear Flow”, by Jim Dufty, Mirim Lee, Jim Lutsko, José Montanero, and Andrés Santos^{6,7}. These papers considered linear perturbations of the density, velocity, and energy fields from the standpoint of the Navier-Stokes-Fourier equations, specialized to small strain rates $\dot{\epsilon}$ and to long wavelengths (or small k vector) normal to the flow direction ($\lambda = 2\pi/k$) . Their analysis showed that for *any* fixed strain rate exponential growth invariably results for perturbations of sufficiently long wavelength.

In early 2012 we chanced upon these contradictory results [*stable* molecular dynamics and *unstable* linear perturbation theory, both for the *same* problem] . To address this puzzle here we first investigated solutions of gas-phase Navier-Stokes-Fourier shear flows with moving periodic images of a square Eulerian continuum grid, using the same periodic-shear boundary conditions illustrated in Figure 1 .

A. Continuum Algorithm for Steady-State Simple Shear

The finite-difference numerical work^{5,8,9} is most naturally carried out for grid space and time differences Δx and Δt chosen near the Courant condition limit, $\Delta t < \Delta x/c$, where c is the fluid's sound speed . The equations to be solved are minor modifications of the usual conservation laws for mass, momentum, and energy :

$$\dot{\rho} = -\rho \nabla \cdot u ; \rho \dot{u} = -\nabla \cdot P ; \rho \dot{e} = -P : \nabla u - \nabla \cdot Q .$$

The boundaries, where the square middle-row cells of Figure 1 contact the upper and lower rows of cells, need to be made consistent with steady shear. Here ρ is the mass density, $u = (u_x, u_y)$ is the velocity, P is the pressure tensor, e the energy per unit mass, and Q the heat flux vector. The superior dots indicate “comoving” “Lagrangian” time derivatives following the motion. An efficient algorithm solving this problem can be based on those

developed for the Rayleigh-Bénard continuum convection problems described in References 5, 8, and 9.

In the continuum periodic-shear algorithm we added a “global” ergostat to the energy equation to constrain the total internal energy. We also added two global “thermostats” to the continuum equations of motion. These thermostats constrained the summed-up squares of the x and y velocity fluctuations to small constant values, relative to the mean simple-shear motion $u_x(y) = \dot{\epsilon}y$. We also included a short-ranged “artificial viscosity” to avoid an “even-odd” instability. The one-dimensional analog of this instability would lead to alternating signs for velocities evaluated at neighboring nodes of a periodic computation mesh with N zones defined by N nodes. At the end of each timestep the i th *nodal* velocity is replaced by a weighted average ($0 < \alpha < 1$) including the *zone* velocities of its neighboring zones :

$$u^n \rightarrow \alpha u_i^n + (1 - \alpha)(u_i^z + u_{i-1}^z)/2 .$$

The two-dimensional periodic shear problem is implemented with densities evaluated in N computational square $\Delta x \times \Delta x$ zones with velocities and energies evaluated at the nodes defining the four corners of the zones. Fourth-order Runge-Kutta integration of the $4 \times N = 4L^2$ ordinary finite-difference equations results in a natural strain rate ,

$$\dot{\epsilon} = 2\Delta x/(L\Delta t) .$$

The factor 2 reflects the two increments of time occurring in a single Runge-Kutta time step. This strain rate is of the same order as the k vector describing the longest-wavelength perturbation :

$$k \equiv (2\pi/L) \simeq \pi\dot{\epsilon}(\Delta t/\Delta x) \simeq \pi\dot{\epsilon}/c ,$$

and is also fairly close to the critical wavelength of the instability analyses.

B. Typical Numerical Results for Continuum Shear of a Gas

A typical 512×512 zone simulation, with

$$[\Delta x = 1 \rightarrow L = 512 ; \Delta t = 0.25 \rightarrow \dot{\epsilon} = 2\Delta x/(L\Delta t) = (1/64)] ;$$

$$[(PV/NkT) = (E/NkT) = 1 \rightarrow c = \sqrt{2} ; \nu = (\eta/\rho) = \rho = \eta = \kappa = 1 ; \eta_V = 0] ,$$

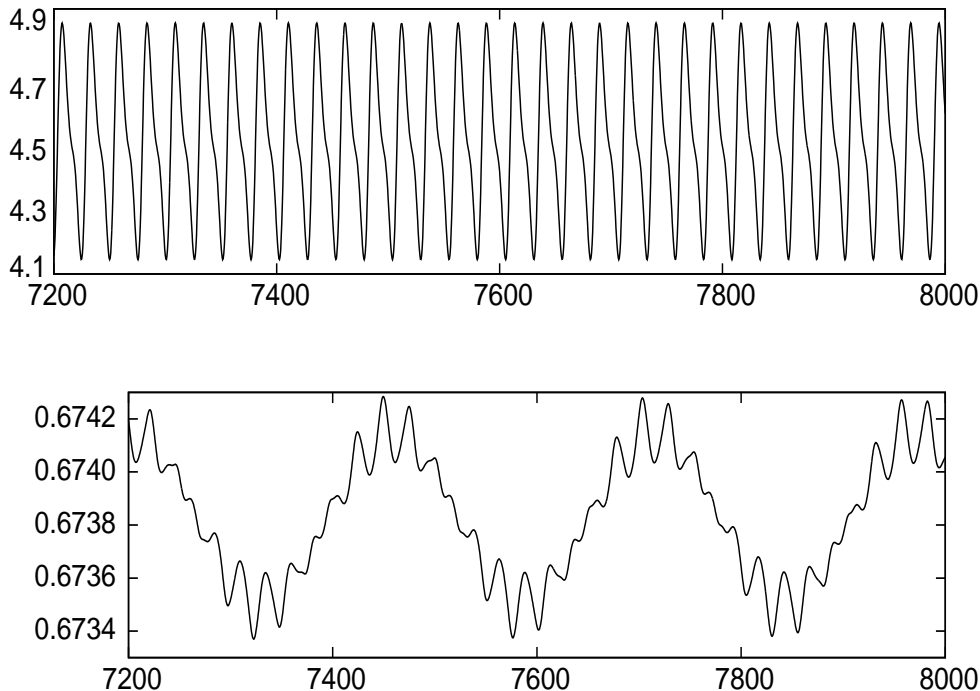


Figure 2: Time history of the horizontal kinetic energy, which includes the single-cell contribution of the shear to the kinetic energy (below) and the much smaller vertical kinetic energy (above) in a square 32×32 Eulerian unit cell. The vertical kinetic energy scale has been multiplied by 10^8 . The strain rate is $\dot{\epsilon} = (2\Delta x/\Delta t)/L = (2/(1/2))/32$. A portion of the time history corresponding to strains from 900 to 1000 is shown. The transport coefficients, density, and internal energy, $\{ \eta, \kappa, \rho, e \}$, are all equal to unity. The Reynolds Number is $R = 4 \times 32 = 128$.

corresponds to a shear flow with a Reynolds' number

$$R = L^2 \dot{\epsilon} / \nu = 512 \times (512/64) / \nu = 4096 ,$$

and is perfectly stable, for a run time of 256×50 steps of 0.25 each, corresponding to a total shear of 50.

We carried out a variety of simulations. Time-dependent data from one of them are shown in Figures 2 and 3. The kinetic energy history, after an irregular transient, is typical, with nearly periodic oscillations of the horizontal and vertical velocity deviations from simple shear flow [these deviations are rescaled at the conclusion of each timestep]. The deviations are analogous to thermal fluctuations. Figure 3 shows these same fluctuations as arrows. These patterns are not stationary, but vary with time. Because the time periodicity of

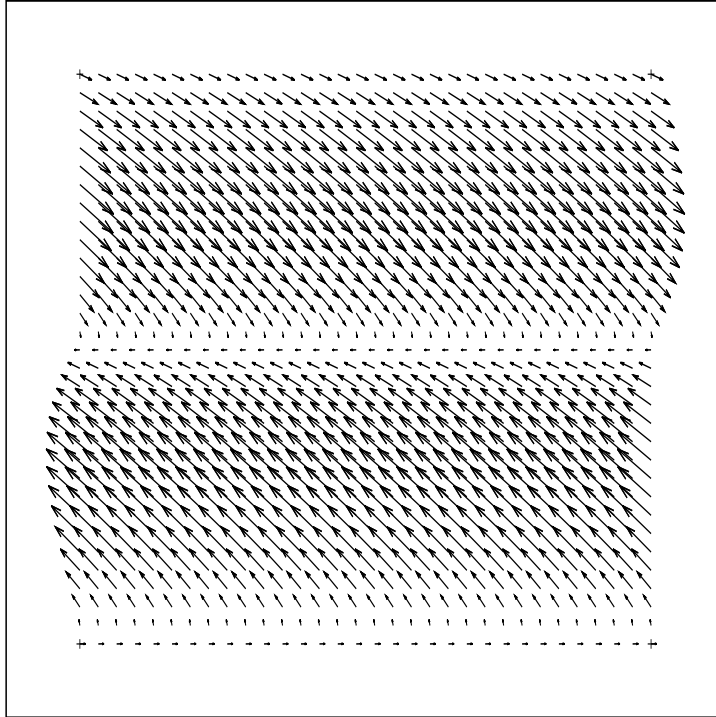


Figure 3: The velocity, relative to the mean flow, $\dot{x} = \dot{\epsilon}y$ for the 32×32 grid described in Figure 2. Although this velocity perturbation is not stationary – it changes with time – this view is typical.

the shear, with period $\tau = (1/\dot{\epsilon})$, is built into the boundary conditions an inhomogeneous perturbation flow is to be expected.

We explored systems with $L \times L$ computational zones, with $L = 8, 16, 32, 64, 128, 256,$ and 512 to strains of at least 100 . With $\Delta x = 1$ and $\Delta t = (1/2)$, so that the Reynolds number is $R = 4L$, all members of this series were stable, giving results similar to those in Figures 2 and 3. Somewhat larger or smaller values of Δt typically led to instability, making it difficult to validate the stability work of References 6 and 7.

These exploratory calculations could be extended in *many* arbitrary ways. We chose instead to follow and extend the linear perturbation-theory hard-sphere work of Dufty *et alii*^{6,7} directly to a numerical model based on our earlier soft-disk shear-flow model. Our results, described in what follows, suggest that the linear perturbation analysis yields flawed predictions, contradicted by the well-established stability of thermostated simple shear in two space dimensions²⁻⁴. Despite our efforts to extend the perturbation analyses, described below, a convincing theoretical demonstration of this finding remains a challenging research goal. It seems likely that the flaw in the perturbation treatment is an inadequate treatment

of steady-state thermostating. Our checks of the other aspects of the perturbation theory have so far revealed no errors.

III. CONSTITUTIVE MODEL FOR SOFT DISKS

The short-ranged repulsive potential $\phi(r < 1) = 100(1 - r^2)^4$ has been carefully investigated near the reference state, $[\rho = 1 ; e = 1]$, where e is the energy per particle and each particle has unit mass³. The equilibrium temperature and pressure at that state are approximately $T = 0.69$ and $P = 3.90$. For our numerical stability studies we adopt the equation of state from Reference 3 :

$$P/\rho = 5 + 8(\rho - 1) + 2.5(e - 1.443) + 9(\rho - 1)^2 + 2(\rho - 1)(e - 1.443) ;$$

$$T = 1 - (\rho - 1) + 0.7(e - 1.443) - 0.8(\rho - 1)^2 - 0.5(\rho - 1)(e - 1.443) ;$$

$$e - 1.443 = 1.5(\rho - 1) + 1.5(T - 1) + 2.4(\rho - 1)^2 + 1.2(\rho - 1)(T - 1) .$$

We estimate the transport coefficients (and evaluate their density and temperature derivatives numerically) η , η_V , κ from Enskog's theory^{10,11}.

Enskog suggested that transport properties for soft potentials be estimated from those of a corresponding hard-potential model. The equivalence is based on setting the soft model's "thermal pressure", $T(\partial P/\partial T)_V$, equal to the hard-potential pressure. In our two-dimensional implementation the hard-disk model corresponding to the soft-disk potential $\phi = 100(1 - r^2)^4$ follows from the relation :

$$(V/Nk)(\partial P/\partial T)_{\text{soft}} \equiv (PV/NkT)_{\text{hard}} .$$

For the hard-disk compressibility factor we use the ten-term virial series from Clisby and McCoy's work¹⁰ :

$$\begin{aligned} [(\partial P/\partial T)/\rho]_{\text{soft}} \equiv (P/\rho T)_{\text{hard}} &= 1 + (b\rho)\chi = 1 + b\rho + 0.782(b\rho)^2 + 0.532(b\rho)^3 + \\ &0.334(b\rho)^4 + 0.199(b\rho)^5 + 0.115(b\rho)^6 + 0.065(b\rho)^7 + 0.036(b\rho)^8 + 0.020(b\rho)^9 + \dots . \end{aligned}$$

Here χ is the ratio of the actual hard-disk collision rate from the virial series to the low-density kinetic-theory collision rate calculated with the two-term series. The computed value of the hard-disk second virial coefficient $b = \pi\sigma^2/2$ gives the hard-disk diameter $\sigma = \sqrt{2b/\pi}$ needed for the hard-disk transport coefficients.

David Gass kindly worked out formulæ for the Navier-Stokes-Fourier transport coefficients for hard disks in 1970¹¹ :

$$\eta = \eta_0 b \rho [(b \rho \chi)^{-1} + 1.0 + 0.8729(b \rho \chi)] ; \eta_V = 1.246 \eta_0 b \rho (b \rho \chi) ; \eta_0 = \sqrt{m k T / \pi} / 2 \sigma ;$$

$$\kappa = \kappa_0 b \rho [(b \rho \chi)^{-1} + 1.5 + 0.8718(b \rho \chi)] ; \kappa_0 = 2 \sqrt{k^3 T / m \pi} / \sigma .$$

These expressions provide estimates for the soft-disk transport coefficients needed to apply the perturbation theory described in the following Section.

IV. DUFTY-LEE-LUTSKO-MONTANERO-SANTOS' LINEAR THEORY

Consider the reference steady shear flow state for soft disks at unit density and energy :

$$\{ \rho = 1 , u_x = \dot{\epsilon} y , u_y = 0 , e = 1 \} .$$

There are extensive molecular dynamics simulation data available for strain rates $\dot{\epsilon}$ of 0.10, 0.25, and 0.50 . We apply linear perturbation theory to this problem for a perturbation with components

$$\{ \delta \rho \times e^{i k y + i \omega t} , \delta u_x \times e^{i k y + i \omega t} , \delta u_y \times e^{i k y + i \omega t} , \delta e \times e^{i k y + i \omega t} \} ,$$

where the unperturbed state is steady shear at a mass density and internal energy per particle of unity :

$$\{ \delta \rho = \rho - 1 , \delta u_x = u_x - \dot{\epsilon} y , \delta u_y = u_y , \delta e = e - 1 \} .$$

In addition to the conservation laws we use the Navier-Stokes-Fourier constitutive relations

$$P = [P_{\text{eq}} - \lambda \nabla \cdot u] I - \eta [\nabla u + \nabla u^t] ; Q = -\kappa \nabla T ,$$

with the Gass-Enskog transport coefficients. As usual η is the shear viscosity. Here λ is the difference between the bulk and shear viscosities , $\lambda = \eta_V - \eta$, and κ is the heat conductivity. To a good approximation $\lambda \simeq 0$, so that the bulk and shear viscosities are roughly equal, and about four times less than the heat conductivity :

$$\eta \simeq 1 \simeq \eta_V = \lambda + \eta ; \kappa \simeq 4 \eta .$$

A. Matrix Solution of the Linear Equations

If we represent the hydrodynamic state perturbations by the four-dimensional vector δ then the linearized hydrodynamic equations take the form of a 4×4 matrix equation, $\dot{\delta} = M \cdot \delta$. Let us begin by estimating the values of the 16 matrix elements. If we (1) ignore the *nonlinear* convective contributions to the equations of motion and (2) assume a solution of the form $\exp[iky + i\omega t]$ we get a set of four *linear* equations for the evolution, in space and time, of perturbations in mass, momentum, and energy :

$$[\text{mass conservation}] : \dot{\rho} = -\rho \nabla \cdot u \longrightarrow$$

$$(\partial \delta \rho / \partial t) \equiv i\omega \delta \rho = -\rho (\partial \delta u_y / \partial y) \equiv -ik\rho \delta u_y ;$$

$$[x \text{ momentum conservation}] : \dot{u}_x = -\dot{e} \delta u_y - (1/\rho) (\partial P_{xy} / \partial y) \longrightarrow$$

$$\begin{aligned} i\omega \delta u_x &= -\dot{e} \delta u_y - (1/\rho) (\partial / \partial y) [-\eta (\partial / \partial y) (\dot{e} y + \delta u_x)] \simeq \\ &-\dot{e} \delta u_y + ik(\dot{e}/\rho) [(\partial \eta / \partial \rho)_e \delta \rho + (\partial \eta / \partial e)_\rho \delta e] - (\eta/\rho) k^2 \delta u_x . \end{aligned}$$

$$[y \text{ momentum conservation}] : \dot{u}_y = -(1/\rho) (\partial P_{yy} / \partial y) \longrightarrow$$

$$\begin{aligned} i\omega \delta u_y &= -(1/\rho) (\partial / \partial y) [P_{eq} - (\eta + \eta_V) (\partial u_y / \partial y)] \simeq \\ &-(ik/\rho) [(\partial P_{eq} / \partial \rho)_e \delta \rho + (\partial P_{eq} / \partial e)_\rho \delta e] - (\eta + \eta_V) k^2 \delta u_y . \end{aligned}$$

$$[\text{energy conservation}] : \dot{e} = (-1/\rho) [P : \nabla u + \nabla \cdot Q] =$$

$$\begin{aligned} &-(1/\rho) [P_{xy} (\partial u_x / \partial y) + P_{yy} (\partial u_y / \partial y) + (\partial Q_y / \partial y)] \longrightarrow \\ &i\omega \delta e \simeq \dot{e}^2 [(\partial \nu / \partial \rho)_e \delta \rho + (\partial \nu / \partial e)_\rho \delta e] + 2ik\nu \dot{e} \delta u_x \\ &\quad - ik(P_{eq}/\rho) \delta u_y - k^2(\kappa/\rho) \delta T . \end{aligned}$$

Note that the kinematic viscosity, $\nu \equiv (\eta/\rho)$ has been introduced in the energy conservation expression. For computation of the matrix elements, and their eigenvalues, it is necessary to express $\nabla^2 T$ in terms of $\delta \rho$ and δe :

$$\delta T = -0.78\delta \rho + 0.7\delta e \longrightarrow \nabla^2 T \simeq k^2 [0.78\delta \rho - 0.7\delta e] .$$

A numerical evaluation of the eigenvalues for a dense grid of k -vectors and strain rates gives two unstable (positive real part, leading to exponential growth) eigenvalues in the shaded

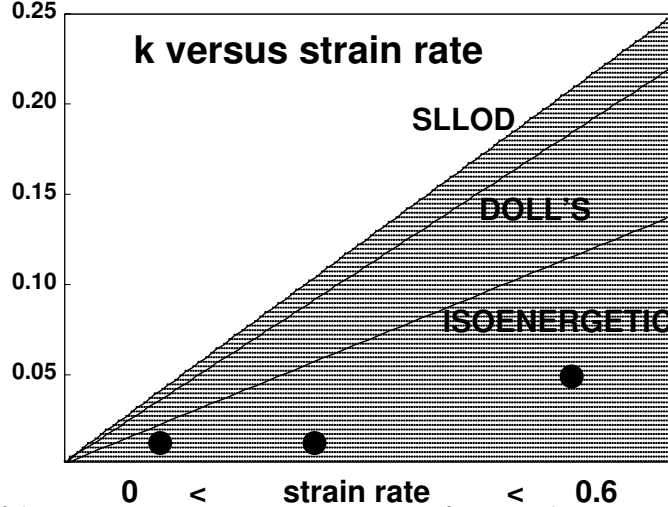


Figure 4: Portion of k -vector *versus* strain rate space for two-dimensional soft disks. Flows in a lower triangular region [shading shows that region for the Sllod Matrix] are *unstable*, leading to longtime exponential growth of perturbations, according to the theory outlined in References 6 and 7. Stable atomistic simulations for soft disks have been carried out for the conditions corresponding to the three filled circles (as well as for *many* other situations). The two approaches to stability give contradictory results. The straightforward nature of the molecular dynamics argues that the perturbation-theory results are invalid.

lower-triangular region shown in Figure 3 (which closely resembles the behavior found by Dufty *et alii*). Notice that the stable large-system molecular dynamics data from References 3 and 4, shown also in the Figure, lie squarely inside the “unstable region”.

The contradiction between perturbation theory and molecular dynamics is robust. We have investigated several modifications of the basic theory and found qualitatively similar results. Replacing the “Sllod” matrix element with its “Doll’s-Tensor” analog,

$$\{ M_{u_x, u_y} = -\dot{\epsilon} ; M_{u_y, u_x} = 0 \} \longleftrightarrow \{ M_{u_x, u_y} = 0 ; M_{u_y, u_x} = -\dot{\epsilon} \} ,$$

leaves the qualitative picture unchanged. Reducing the matrix to 3×3 by ignoring the possibility of energy fluctuations still yields an unrealistic triangular “unstable region”. We have no explanation for the failure of perturbation theory to deal with steady simple shear.

V. CONCLUSION

Although the evidence from molecular dynamics supports the large-system stability of thermostated steady shear, linear stability analysis, with a fixed global thermostat, predicts

instability. Where might the explanation lie? We don't know. Explanations might involve either of two flow features treated poorly by the theory: [1] The “steady-state” shear flow is not really stationary. See again Figure 2. At times which are integral multiples of the inverse shear rate, $t = n(1/\dot{\epsilon})$, the periodic arrangement of cells is a perfect rectangular checkerboard; [2] Evidently the molecular dynamics thermostats provide additional stability to the flow.

A variety of molecular dynamics algorithms, with thermostats or with ergostats and with Doll's or Sllod equations of motion, all give very similar results, all of them identical for the *linear* response proportional to $\dot{\epsilon}$. It may be that some more faithful representation of the thermostat forces in the perturbation theory could lead to results consistent with the molecular dynamics. We would be most grateful for an explanation of the apparent contradiction between the atomistic and continuum approaches to the stability of steady two-dimensional “simple shear”.

It seems to be an accepted result (though the exact assumptions required are unclear) that *linear* stability theory predicts stability for simple shear at *all* Reynolds numbers. See, for instance, Reference 12. On the other hand the necessary *inhomogeneity* due to the boundary conditions, and the need for thermostat and/or ergostat heat sinks, provide opportunities for a wide variety of much more complex models for this “simple” shear problem.

VI. ACKNOWLEDGMENT

Bill thanks Andrew Gabriel De Rocco for arranging a meeting with Peter Debye *circa* 1960. Debye's advice, to choose research topics from among existing puzzles in the literature, has been an enduring guide. We are looking forward to discussing the present work at the 40th Summer School, “Advanced Problems in Mechanics” at Saint Petersburg in Summer 2012 .

VII. ADDENDUM OF 24 APRIL 2012

We wish to thank Vitaly Kuzkin for emphasizing the relevance of Denis Evans and Gary Morriss' paper, “Nonequilibrium Molecular Dynamics Simulation of Couette Flow in Two-Dimensional Fluids”, Physical Review Letters **51**, 1776-1779 (1983). Evans and Morriss

studied the shear viscosity of 896 and 3584 soft-disk particles at several strain rates and densities. Just as in our work in References 1-5 they observed only a small number dependence, and a nearly rate-independent viscosity rather than the divergence of viscosity predicted by the mode-coupling models. Their viscosity data look closely Newtonian, so long as the strain rate is not too large. In 1983 this was a surprise as the mode-coupling models of the 1970s current then predicted the *divergence* of viscosity in two-dimensional fluids. Influenced by those models, Evans and Morriss explained the observed unexpected stability of their own results as a “screening instability” due to transverse velocity fluctuations. By removing the three longest-wavelength fluctuations Evans and Morriss recovered a logarithmic rate-dependence, $\eta \simeq \ln(1/\dot{\epsilon})$. They commented that larger systems would require the removal of even more Fourier components of the transverse velocity fluctuations in order to squelch their observed Newtonian behavior.

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