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12-27-82

UCRL-88315
PREPRINT
Conf-821014--1

MASTER

UCRL--88315

DE83 004303

RHEOLOGY VIA NONEQUILIBRIUM MOLECULAR DYNAMICS

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This paper was prepared for presentation at
Annual Meeting of the Society of Rheology,
Evanston, Illinois on October 27, 1982

October 1982

Lawrence
Livermore
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RHEOLOGY VIA NONEQUILIBRIUM MOLECULAR DYNAMICS [1]

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Abstract

The equilibrium molecular dynamics formulated by Newton, Lagrange, and Hamilton has been modified in order to simulate rheological molecular flows with fast computers. This modified "Nonequilibrium Molecular Dynamics" (NEMD) has been applied to fluid and solid deformations, under both homogeneous and shock conditions, as well as to the transport of heat. The irreversible heating associated with dissipation could be controlled by carrying out isothermal NEMD calculations. The new isothermal NEMD equations of motion are consistent with Gauss' 1829 "Least-Constraint" principle as well as certain microscopic equilibrium and nonequilibrium statistical formulations due to Gibbs and Boltzmann. Application of isothermal NEMD revealed high-frequency and high-strain-rate behavior for simple fluids which resembled the behavior of polymer solutions and melts at lower frequencies and strain rates. For solids NEMD produces plastic flows consistent with experimental observations at much lower strain rates. The new nonequilibrium methods also suggest novel formulations of thermodynamics in nonequilibrium systems and shed light on the failure of the "Principle of Material Frame Indifference."

Introduction

Newton's and Fourier's linear formulations of viscous flow and heat flow have long served as useful descriptions of monatomic simple-fluid behavior. At least for gases, the basic physics of these linear theories was well understood by the close of the 19th century. At that time, Boltzmann's transport equation, soon to be solved by Chapman and Enskog [2], gave a quantitative explanation of Newtonian gas viscosity and Fourier's heat conductivity.

For more complicated molecular or polymeric fluids, particularly lubricants, deviations from Newtonian viscous flow have been abundantly documented in the 20th century, since Boltzmann's day. Very recently, advances in computer technology have made it possible to simulate these deviations via nonequilibrium molecular dynamics (NEMD), reproducing nonlinear non-Newtonian effects observed experimentally. NEMD has even been able to show that now-Newtonian effects occur for the very simplest materials at high rates of strain.

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Nonlinear problems, and their simulation using computers, are attracting attention in many places--Australia, Belgium, England, France, Holland, Italy, Japan, Russia, and the United States [3]. The main goal of this modern research is to make a quantitative connection between the microscopic interatomic and intermolecular force laws and observed macroscopic rheological laws.

Of course the many-body correlations present in dense fluids and solids are contained in the fundamental dynamical equations of Newton, Lagrange, and Hamilton. So why has it taken so long to apply these equations to rheological problems? Straightforward application is limited by computer hardware to relatively short (nanoseconds) and small (millimicrons) problems. These calculations are further complicated by small-system boundary effects and by the relatively large size of statistical fluctuations. It has taken time to develop methods circumventing these problems.

In the last decade, nonequilibrium molecular dynamics has begun to simulate steady homogeneous flows in the absence of physical boundaries. The NEMD methods, which are based on modifications of the equations of motion to include dynamical constraints, are beginning to be applied to polyatomic molecules of rheological interest. Here we describe results obtained so far for relatively simple central-force models. We forecast the possibilities for calculations in the next few years.

Because computational advances have outstripped theoretical ones, the theoretical side of nonlinear transport in dense fluids and solids is wide open. The effects found in relatively straightforward computer simulations deviate substantially from theoretical predictions. It is not clear why this is so or how the theory will come to terms with the new results [4]. In rheology it is taken for granted that material behavior can be nonanalytic. This assumption is less common in microscopic physics, but certainly is strongly suggested by some theoretical approaches and the new computer experiments.

Equilibrium Molecular Dynamics

Equilibrium molecular dynamics was developed by Alder, Rahman, Verlet, Vineyard, and their co-workers [5-8]. The main goals of molecular dynamics are (1) characterizing the approach to equilibrium, (2) characterzing equilibrium, and (3) characterizing reproducible nonequilibrium phenomena. In every case a correspondence must be established between the microscopic view of matter, based on Newton's, Lagrange's, or Hamilton's equations, and the phenomenological kinetic and constitutive equations of continuum mechanics. The microscopic laws are typified by Newton's "Equation of Motion":

$$m\ddot{q} = F \ . \tag{1}$$

The macroscopic analog, for a material with a pressure tensor P, a density ρ, and a stream velocity u, is the continuum "Equation of Motion"

$$\rho\dot{u} = -\nabla\cdot P \ . \tag{2}$$

Newton's microscopic equations are incomplete in the sense that the boundary conditions need to be specified in detail before nonequilibrium problems can be attacked. The macroscopic equations are likewise incomplete. The "Constitutive Relations" relating the pressure tensor, temperature, and heat flux to the strain-rate tensor and the temperature gradient, must be given to specify a well-posed problem. The constitutive relations are usually imagined to come from clever experiments. The ambition of a molecular-level theorist is to circumvent the laboratory and find the constitutive properties using microscopic equations of motion instead.

To link the microscopic and macroscopic points of view it is first necessary to formulate microscopic analogs of the continuum macroscopic variables: temperature, energy, the pressure tensor, and so on. The formulation of Irving and Kirkwood [9] is the usual basis for these definitions. Temperature, for instance, is related to the mean-squared velocity relative to the local stream velocity:

$$(3/2)kT = (1/2)m\langle(v-u)^2\rangle \ . \tag{3}$$

Trajectories governed by the equilibrium equations of motion (1) are easily generated. The early calculations [5-8] solved these coupled equations for up to several hundred particles, and successfully characterized the approach to equilibrium and the equilibrium equation of state. The linear transport coefficients were also obtained from the Green-Kubo linear response theory [10]. The equilibrium results--pressure and temperature as functions of energy and volume--agreed well with the Los Alamos Monte-Carlo estimates--pressure and energy as functions of volume and temperature--based on Gibbs' statistical mechanics [11-12].

The early thermodynamic results showed that deviations from the large-system thermodynamic limit can be as small as 1/N or (lnN)/N, provided that periodic boundary conditions are used to eliminate surface effects [13]. Thus a reasonable equilibrium equation of state can be obtained with only 100 particles.

About ten years later in 1969, perturbation theories were developed [14] which made it possible to calculate, by using known hard-sphere functions, the equations of state for "simple fluids" with pairwise-additive forces. It became possible to generate complete phase diagrams for these simple fluids by perturbation theory, without further simulations. The equilibrium properties of simple fluids became a "mature" field.

The linear nonequilibrium properties are a remaining challenge. The straightforward nonequilibrium perturbation theory doesn't seem to converge [15], and the Green-Kubo calculations are both time-consuming and imprecise.

Evolution of Nonequilibrium Molecular Dynamics

To verify linear viscosities and conductivities, and to explore nonlinear transport, the equilibrium work had to be generalized. It was necessary to formulate boundary conditions, or altogether new equations of motion, to measure nonlinear effects: How does the viscosity vary with strain rate? How does thermal conductivity vary with temperature gradient? How are the momentum and heat currents coupled together? Dealing with the nonlinear problems was a two stage process. The first stage was to use special boundaries [16-17] or external fields [18] to maintain local temperatures or velocities. This work showed that experimental viscosities and conductivities could be reproduced, with uncertainties on the order of several percent, by several independent methods. The next stage was the development of more efficient calculational methods, to reduce the uncertainties, for application to nonlinear problems. The two major obstacles were (1) the relatively large influence of physical boundaries and (2) the nonsteady increases in temperature and pressure caused by irreversible heating. Both difficulties have been eliminated by using clever nonequilibrium schemes.

At first, moving physical boundaries were used to drive viscous shear and dilatational flows. These were later eliminated by using time-dependent periodic boundaries in conjunction with equations of motion which reproduced the desired macroscopic flow fields [19]. The simplest case is plane Couette flow, with the x component of stream velocity proportional to y. A "Doll's Tensor" Hamiltonian, formed by adding the microscopic velocity (p_x/m) to the stream velocity $\dot{\epsilon} y$, reproduces the macroscopic flow field and also generates new momentum-dependent Coriolis' forces:

$$H = H_o + \dot{\epsilon} \sum y p_x \; ; \quad H_o = \Phi + \sum (p^2/2m) \; ; \tag{4}$$

$$\dot{x} = (p_x/m) + \dot{\epsilon} y \; ; \quad \dot{y} = (p_y/m) \; ; \tag{5}$$

$$\dot{p}_x = F_x \; ; \quad \dot{p}_y = F_y - \dot{\epsilon} p_x \, . \tag{6}$$

The set of Doll's-tensor equations of motion derived from (4) can be shown to reproduce identically the first law of thermodynamics for Couette flow:

$$\dot{E} \equiv -\dot{\varepsilon} V P_{xy} , \tag{7}$$

where the energy E and the pressure-tensor component P_{xy} are the instantaneous values of fluctuating microscopic variables. The moving boundaries used in conjunction with these nonequilibrium equations of motion are identical to those of Lees and Edwards [16]. A variant of these boundaries, in which periodic images move toward the central periodic cell, can be used to simulate shockwaves [20].

Heat conduction could not be handled in such a straightforward way. To generate a heat current in a homogeneous periodic system an external force linear in the energy (pushing energy-rich particles to the right and energy-poor particles to the left) had to be developed [21]. Once this was done, both deformation and heat current could be simulated in small periodic systems.

What about the irreversible heating? This was a potentially serious problem, because large gradients are required in order to measure a statistically well-defined response. The heating leads to thermodynamic changes of state. In Ashurst's original calculations reservoir regions were maintained at constant temperatures by rescaling the velocity distribution, relative to its mean, to maintain a constant second moment. This same end can be achieved, more elegantly, by imposing a "nonholonomic" (i.e., involving velocities, not just coordinates) constraint on the motion:

$$(d/dt) \sum (p^2/2m) = 0 . \tag{8}$$

If the constraint is arbitrarily imposed by adding to each particle an acceleration proportional to its momentum:

$$\Delta\dot{p} = -\zeta p \; , \tag{9}$$

then the (time-dependent) friction coefficient ζ can be given as an explicit function of the interparticle forces and the momenta:

$$\zeta = \sum F\cdot p / \sum p\cdot p \; . \tag{10}$$

With both the artificial boundaries and the irreversible heating removed, it became possible to study steady nonlinear flows, with large gradients, for the long times necessary to obtain good statistics. The main unresolved question then was: would the computer calculations correspond to laboratory experiments?

Is NEMD Legitimate Physics?

Do the NEMD simulations correspond to physical reality? One way to approach this question is empirical. Calculations can be carried out with different constraints. For instance, constant temperature or constant energy or constant pressure constraints could be imposed on a system undergoing shear deformation. To the extent that the resulting shear stress is independent of the constraint type, it is at least plausible that the measured stress-strain rate relation is physically correct. Evans carried out such an investigation, comparing shear stresses under conditions of constant temperature and constant energy. The two simulations agreed within the relatively small shear stress fluctuations [22].

It is also possible to analyze some of the NEMD methods theoretically. The isothermal dynamics used by Ashurst, for instance, can be simply related to Gauss' variational principle of least constraint [23]. Gauss believed that the trajectory observed, in a constrained system, would be that which minimized the mean-squared change in the particle accelerations due to the constraints:

$$\sum m(\delta\ddot{q})^2 = \text{minimum.} \tag{11}$$

If this minimization is carried out under the constraint of fixed kinetic energy then exactly Ashurst's velocity-rescaling scheme results. The same isothermal NEMD calculations can also be related to Gibbs' equilibrium ensemble studies [24]. Gibbs proved that the most likely distribution for a fixed-temperature fixed-volume system is one in which the state probability varies as $\exp(-E/kT)$. It is interesting that isochoric NEMD equations of motion which fix T, but allow E to vary, identically reproduce Gibbs' canonical distribution if that distribution is chosen initially.

It is also possible to connect NEMD with low-density nonequilibrium theory [25]. Boltzmann showed how to treat the collisional evolution of nonequilibrium systems by computing the single particle distribution function $f(q,p)$. In the case that the only nonvanishing component of the strain-rate tensor is $\dot{\varepsilon} = du_x/dy$, Chapman and Cowling's results show [26] that the shear and normal stresses, for Maxwell molecules, are

$$P_{xy}V/NkT = -\dot{\varepsilon}\tau + O(\dot{\varepsilon}\tau)^3 ;$$

$$P_{xx}V/NkT - 1 = +(4/3)(\dot{\varepsilon}\tau)^2 + O(\dot{\varepsilon}\tau)^4 ;$$

$$P_{yy}V/NkT - 1 = -(2/3)(\dot{\varepsilon}\tau)^2 + O(\dot{\varepsilon}\tau)^4 ;$$

$$P_{zz}V/NkT - 1 = -(2/3)(\dot{\varepsilon}\tau)^2 + O(\dot{\varepsilon}\tau)^4 , \qquad (12)$$

where the "collision time" τ is of the order of the time between collisions. The system gradually heats up: $d\ln T/dt = (2/3)\dot{\varepsilon}^2 \tau$.

How must these results be modified if the isothermal NEMD restriction is imposed, so that temperature is fixed? This situation can be analyzed from the viewpoint of the relaxation-time model of the Boltzmann equation [10]:

$$(\partial f/\partial t) = -d(\dot{q}f)/dq - d(\dot{p}f)/dp + (f_o - f)/\tau , \qquad (13)$$

where f_o is the local equilibrium distribution:

$$f_o = (N/V)\exp(-p^2/2mkT)/(2\pi mkT)^{3/2} . \qquad (14)$$

If f is expanded as a power series in the collision time, $f = f_o + \tau f_1 + \tau^2 f_2 + \ldots$ then the equations of motion,

$$
\begin{aligned}
\dot{x} &= (p_x/m) + \dot{\varepsilon} y \;; \\
\dot{y} &= (p_y/m) \;; \\
\dot{z} &= (p_z/m) \;; \\
\dot{p}_x &= F_x - \dot{\varepsilon} p_y - (\dot{\varepsilon}^2 \tau/3) p_x \;; \\
\dot{p}_y &= F_y - (\dot{\varepsilon}^2 \tau/3) p_y \;; \\
\dot{p}_z &= F_z - (\dot{\varepsilon}^2 \tau/3) p_z \;; \qquad (15)
\end{aligned}
$$

are consistent with (13) if

$$f_1/f_o = -\dot{\varepsilon}[p_x p_y/mkT] \,,$$

$$f_2/f_o = \dot{\varepsilon}^2[(p_x p_y/mkT)^2 - ((p_x^2 + 4p_y^2 + p_z^2)/3mkT) + 1] \,. \qquad (16)$$

It is easily verified that this steady-state isothermal NEMD distribution function (16) reproduces the known exact pressure tensor (12).

Results so far Obtained from NEMD

The first NEMD results [16-18] established that computed linear viscosities and heat conductivities agreed with experiment. Work on the nonlinear frequency and amplitude dependence of the transport coefficients can not so easily be compared with experiment because very high rates are involved. It is necessary that neighboring particles move at a non-negligible velocity, relative to the sound speed, in order for the small-system shear stress to exceed background fluctuations. It was therefore extremely interesting to find [27] that the solid-phase power-law dependence of stress on strain rate established in NEMD simulations at very high rates could be extrapolated, over four orders of magnitude in strain rate, to give satisfactory agreement with experimentally-measured plastic flows. The extrapolation and the experimental data are both somewhat uncertain, but the good agreement suggests an underlying simplicity in the flow mechanism over a wide range of rates.

Similar agreement will probably result for liquids. It has long been known that Maxwell's relaxation-time model of viscoelasticity is an oversimplification for large molecules. Lamb[28] has presented a corresponding states plot of the real and imaginary parts of the shear impedance as functions of frequency for a variety of large molecules. The frequency-dependent viscosity derived from these curves deviates substantially from the Maxwellian model, but resembles much more closely [4] corresponding calculations carried out by Evans [29] for a simple central-force model at much higher frequencies.

Hanley and Evans have considered the nonequilibrium thermodynamics of systems undergoing shear [30]. Analogs of the thermodynamic Maxwell relations, but involving the strain rate as an independent variable, were developed and checked numerically. This thermodynamic work made it possible to evaluate the shift in equilibrium phase diagrams induced by shear. With the development of this theory there is motivation to characterize phase-diagram shifts experimentally.

Finally the Principle of Material Frame Indifference, notoriously hard to test in laboratory experiments due to the high angular velocities involved, can readily be tested in computer experiments. These computer experiments established that high rotational speeds cause an angular heat flow in response to a radial temperature gradient, a violation of Fourier's law which is easily understood from the point of view of the Boltzmann equation [31].

What Lies Ahead?

Work in progress suggests that new results will emerge at an accelerating pace over the next few years. Groups working on larger molecules, butane [32] and decane [33], as well as platelike and rodlike molecules capable of undergoing smectic and nematic liquid-crystal phase transitions [34] should begin to assess the importance of molecular shape to rheological nonlinearities. Work is also in progress on the simulation of granular materials, a promising potential application of NEMD where a variety of interesting experimental data already exists [35]. The possibility of transverse displacement of periodic images, with a superimposed constant normal force, suggests that solid-phase coefficient of friction measurements could also be carried out.

The generalization of the results obtained so far to the more complicated molecular models should proceed smoothly. This should make possible a detailed comparison of microscopic simulations with the mesoscopic models developed by Bird and his Wisconsin coworkers [36] to describe polymeric systems. These latter models are already firmly linked to experiment, so that the end product of the developing NEMD techniques will be a detailed physical understanding of rheological flows.

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1. This work was supported, at Davis, by the Army Research Office and Electric Power Research Institute and carried out, at LLNL, under the auspices of the Department of Energy, under contract W-7405-ENG-48 with the University of California. Conversations and correspondence with Denis Evans, Jim Dufty, Jim Haile, Tony Ladd, Tom Leete, Bill Moran, and Solveig Shearer were pertinent, stimulating, and helpful.

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