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COMPUTER SIMULATION OF NONEQUILIBRIUM PROCESSES

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Recent atomistic simulations of irreversible macroscopic hydrodynamic flows are illustrated. An extension of Nosé's reversible atomistic mechanics makes it possible to simulate such non-equilibrium systems with completely reversible equations of motion. The new techniques show that macroscopic irreversibility is a natural inevitable consequence of time-reversible Lyapunov-unstable microscopic equations of motion.

1. ATOMISTIC SIMULATIONS OF MACROSCOPIC FLOWS FAR FROM EQUILIBRIUM

Atomistic simulations have been applied to a host of macroscopic problems--fracture, fragmentation, and penetration mechanics[1,2], shockwave compression[3], turbulence[4], and thermally-driven gravitational instability[5]. See Figure 1. Such work can lead to modified macroscopic descriptions which include size- and time-dependent constitutive information (surface tension, viscosity, thermal diffusivity, and the like) for the same atomistic model. Besides the size dependence, the main discrepancy between the atomistic simulations and their macroscopic analogs is the relatively large fluctuation size, of order $N^{-1/2}$. The number of particles N is typically somewhat less than a million.

2. REVERSIBILITY AND LYAPUNOV INSTABILITY OF MICROSCOPIC EQUATIONS OF MOTION

The meaning of reversibility in atomistic equations of motion is clear. If we consider snapshot values of particle coordinates q at times ndt, obtained by integrating the equations of motion, then any set n = 0, ±1, ±2, ±3, ..., satisfying the equations of motion with a positive timestep dt is also a solution with dt negative. It is fascinating that motion equations with this reversibility property underlie the macroscopic irreversibility described by the Second Law of Thermodynamics.

The observed irreversibility of macroscopic flows is a consequence of the microscopic Lyapunov instability inherent in the underlying reversible equations of motion.

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The instability is described in terms of the Lyapunov "spectrum", that is, the set of

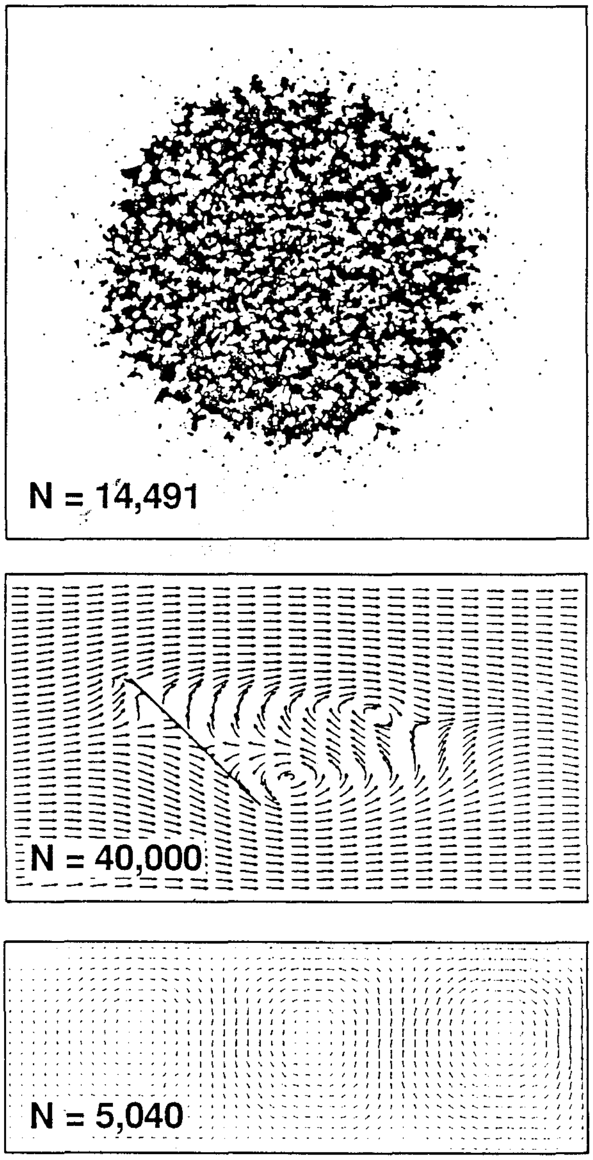

FIGURE 1
Nonequilibrium simulations of fragmentation, turbulence, and Bénard instability. These illustrations are taken from References 1, 4, and 5.

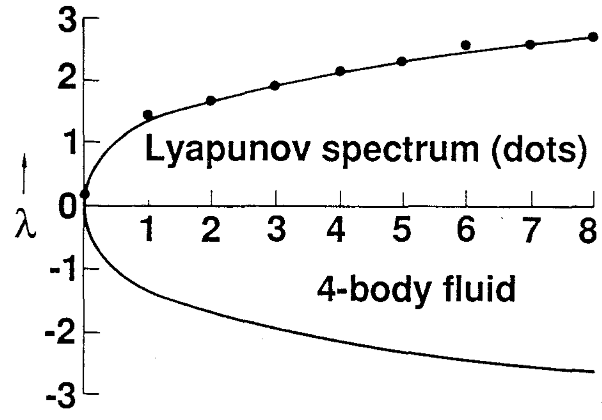

FIGURE 2
Lyapunov spectrum for a 4-body dense fluid. The full curve is a Debye spectrum.

Lyapunov exponents, λ_1, λ_2, λ_3, ... These Lyapunov exponents describe the D orthogonal growth rates of infinitesimal phase-space hypervolumes centered on a moving phase-space trajectory point. The largest Lyapunov exponent describes the exponential growth rate of a one-dimensional "volume"--that is, the rate at which two neighboring phase-space points separate. The sum $\lambda_1 + \lambda_2$ describes the rate at which a two-dimensional area --defined by three neighboring phase-space

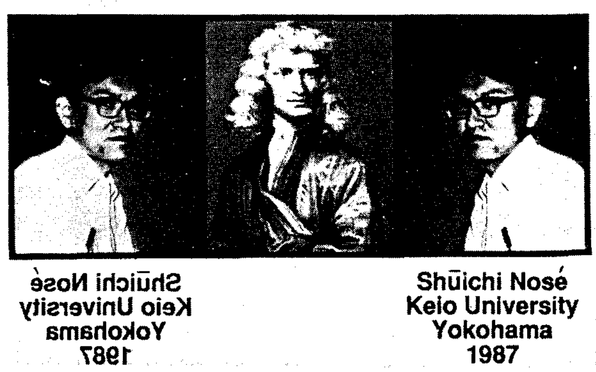

FIGURE 3
Schematic illustration of a far-from-equilibrium Newtonian bulk region driven by two reversible Nosé-Hoover heat revervoirs.

points--grows, and so on. The Lyapunov spectrum has a shape similar to the Debye spectrum of solid state physics[6]. See Figure 2.

Reversible equations of motion describing nonequilibrium systems have been developed recently. Figure 3 shows a bulk Newtonian region driven by two reversible Nosé reservoir regions. To enforce boundary conditions--that is, specifying the temperature, stress, or stream velocity in selected boundary regions --reversible friction coefficients ζ_i are added to the Newtonian equations of motion. For a particle in the ith reservoir region:

$$m\ddot{q} = F(q) - \zeta_i m\dot{q} \; . \quad [\text{Region } i] \qquad (1)$$

In the remaining unconstrained bulk system the usual Newtonian equations of motion, $m\ddot{q} = F(q)$ are used. The complete set of equations of motion, describing the bulk and the boundary regions, is time reversible. In a reversed motion each of the boundary friction coefficients ζ_i changes sign. Three separate derivations[7-9] have been given for this generalization (1) of Newtonian mechanics: (i) They are a consequence of a scaled-time evolution of trajectories following Nosé's canonical-ensemble Hamiltonian. (ii) They are a consequence of the application of Gauss' Principle of Least Constraint to reservoirs constrained to fixed kinetic energy (temperature). (iii) They are the simplest equations of motion which generate the canonical phase-space distribution.

The explicit equilibrium equations (1) were developed by Nosé[7]. The isokinetic Gaussian version had already been applied implicitly much earlier by Ashurst[10] to viscous flows and heat flows. The reversibility of the latter nonequilibrium friction-coefficient equations of motion was first explicitly recognized by Hoover, Ladd, and Moran[8] at about the same time as Nosé's equilibrium work. Independently Denis Evans developed the same nonequilibrium motion equations. Now these same equations are being used primarily to control nonequilibrium simulations of hydrodynamic flow processes.

3. IRREVERSIBILITY OF NONEQUILIBRIUM SYSTEMS

The Nosé-Gauss equations of motion are time-reversible. But, these equations have amazing consequences for nonequilibrium problems. For a system with two or more boundary regions, there are two or more different velocity or temperature constraints, with corresponding friction coefficients, as shown in Figure 3. In what follows we consider two (hot/cold) reservoirs with (N_H/N_C) degrees of freedom, friction coefficients (ζ_H/ζ_C), temperatures (T_H/T_C), and response times (τ_H/τ_C). In this case the Nosé-Hoover Hamiltonian "H" can be proved to be a constant of the motion:

$$\text{"H"} = \sum p^2/2m + \Phi + N_H k T_H(\tau_H\zeta_H)^2/2 + N_C k T_C(\tau_C\zeta_C)^2/2 + \int^t [N_H k T_H \zeta_H + N_C k T_C \zeta_C]dt' \; . \qquad (2)$$

Let us assume the existence of a nonequilibrium steady state, so that the kinetic energy is finite. It follows that the two time integrals in (2), representing the heat transfers at the hot and cold temperatures, cancel. It is also clear that the time-averaged D-dimensional-phase-space-volume strain rate $\langle d\ln V_D/dt \rangle$ cannot be positive in the steady state. This gives the relations

$$\langle d\ln V_D/dt \rangle = \sum \lambda_i = - N_H\zeta_H - N_C\zeta_C < 0. \quad (3)$$

Equations (2) and (3) taken together imply that the hot friction coefficient is negative and the cold one positive, in agreement with the Second Law of Thermodynamics. This very general conclusion follows from the assumed existence of a steady state. An alternative description of this result is that microscopic stability (existence of a steady-state solution of the equations of motion) implies macroscopic stability (positive transport coefficients in agreement with the Second Law of Thermodynamics). It is the deterministic form of the reservoirs that makes it possible to establish this interesting result. Thus the methods designed to model systems far from equilibrium produce, as a fringe benefit, an understanding of the Second Law of Thermodynamics[11].

4. FRACTAL ATTRACTORS AND IRREVERSIBILITY IN NONEQUILIBRIUM FLOWS

From the perspective of Lyapunov instability, the generalized Nosé mechanics suggests the collapse of phase-space probability onto a fractal attractor subspace with dimensionality $D-\delta D$ in a time of order the collision time. Studies of this collapse, for one-body field-driven diffusion[12,13], inspired by equilibrium work on a single one-dimensional oscillator[9,14,15], were sufficiently novel that the first comprehensive descriptions were personally rejected by editors of Physical Review Letters and the Journal of Statistical Physics[16]. That work[12,13] demonstrated that the fractal attractor dimensionality of a steady nonequilibrium state is less than the equilibrium dimension D. Because the volume of a $(D-\delta D)$-dimensional attractor in a D-dimensional space is precisely zero, the volume of the time-reversed repellor (with $p \to -p$ and $\zeta \to -\zeta$) is likewise zero. Thus the probability of observing a repellor state, which would violate the Second Law of Thermodynamics, is exactly zero.

The steady-state attractor's dimensionality loss δD can be estimated:

$$\delta D = \dot{S}/(\lambda_1 k) \ . \qquad (4)$$

λ_1 is the largest Lyapunov exponent and k is Boltzmann's constant. Applied to the Bénard problem at the base of Figure 1 the dimensionality loss would be about 50. The loss δD is extensive, and becomes of order D when the gradients approach those found in strong shockwaves, 10^8/cm for $\nabla \ln T$, and 10^{12} Hz for ∇u.

The applications of these new ideas, and their quantum analogs, are under active investigation. Prospects for nonequilibrium simulation are more exciting than ever before.

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