The Microscopic Approach to Complexity in Non-Equilibrium Molecular Simulations

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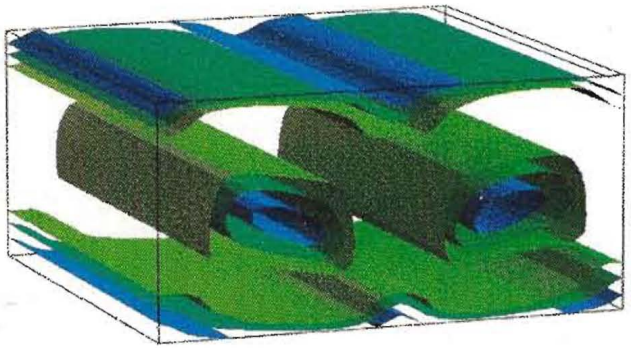

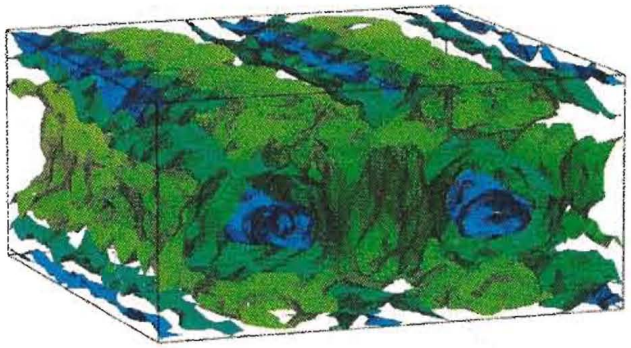

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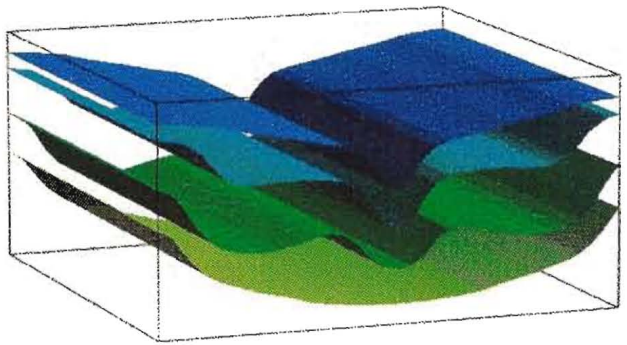

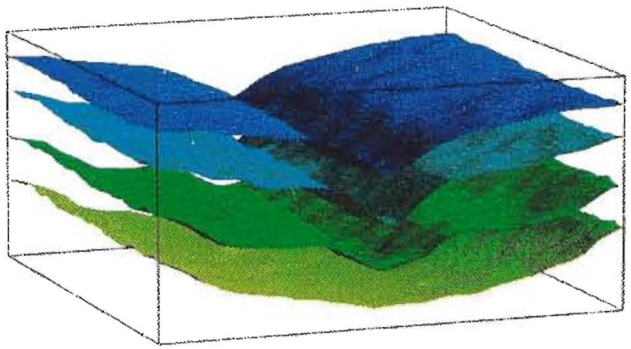

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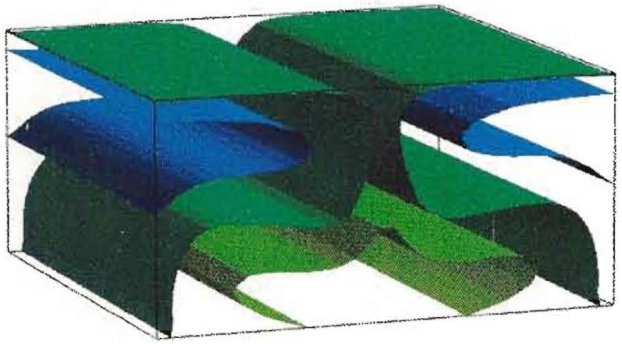

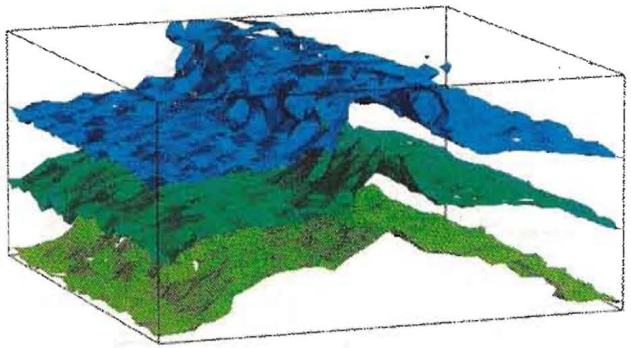

Navier–Stokes

SPAM

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PHYSICA A

Mécanique de Nonéquilibre à la Californienne

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Abstract

Academic freedom, combined with generous travel grants and tax-supported computing, made possible my 35 years' study of many-body problems. Here I first review some of the many high points of those years. I then describe recent work – with Harald Posch, Oyeon Kum, my wife Carol, Siegfried Hess, and Vic Castillo – which links together particle and continuum mechanics through "SPAM", Smooth Particle Applied Mechanics.

1. Introduction

My research has always been chaotic, despite my best-laid plans. I began my graduate work at Michigan by puzzling over what looked like a mistake. Its correction eventually became my dissertation. I next took on an ill-posed problem assigned to me as a fresh postdoc at Duke. Later, as a maturing scientist at the Livermore Laboratory, I repeatedly managed to arrange for research leaves devoted to well-defined projects in Australia, Austria, and Japan. Each project had to support Livermore's "Laboratory Mission", and had to be described in advance in considerable detail. In every case this comprehensive planning was ineffective. I ended up, instead, doing something entirely different, and with someone other than my planned collaborator. Throughout these chaotic stimulating times, and those that followed, I have been sustained, motivated, and entertained by some wonderful people, including the organizers of this meeting, Brad and Michel.

My thesis work at Michigan began with a careful study of one of Bob Zwanzig's few mistakes. I had stumbled across a paper [1] in which he stated that hard-sphere virial coefficients can be bounded by the values of the corresponding parallel-hard-cube ones. It took me a year to feel confident that this was wrong [2]. When my thesis advisor, Andy De Rocco, telephoned Bob to discuss my findings, Zwanzig took only a few seconds to understand, and to agree with, the fruits of my first research effort.

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At Duke, as a fresh postdoc paid at twice the graduate-student rate, I was becoming more efficient. It took only three weeks for me to discover that the set of coupled differential equations given me to solve by Jacques Poirier [3] was internally inconsistent.

At Duke, now unfettered by supervision, I was repeatedly exposed to the unplanned, but common, phenomenon of simultaneous independent discovery. George Stell [4] and I got acquainted through our parallel investigations of hard-particle virial coefficients. Ben Widom discovered a more-general version of my relation [5] linking the hard-particle chemical potential to the pair-distribution function. Carnahan and Starling discovered the same hard-sphere equation of state I had excitedly shown to Andy De Rocco in my student days at Michigan.

After a year at Duke my salary doubled again, for the second and last time, when Berni Alder attracted me to my first real job, at the "Rad Lab" at Livermore. Despite having spent my college and university years as a chemist, I was now officially a physicist. At Livermore I also met Francis Ree and Tom Wainwright. We all collaborated successfully on a variety of hard-particle projects. Kirkwood's single-occupancy idea, coupled with Francis' diligent enthusiasm, soon led to accurate locations for the hard-disk and hard-sphere phase transitions [6]. The subtleties of the hard-disk melting transition continue to attract curious physicists [7].

By 1972 a proliferation of Monte Carlo simulations and the development of perturbation theory had taken the mystery out of equilibrium properties. Further studies of idealized hard disks and spheres did not appeal to me. By then I was familiar with Rahman's work [8]. Its simplicity and elegance persuaded me that molecular dynamics with continuous potentials was well worth learning, and doing. Bill Ashurst was willing to work with me and eager to simulate nonequilibrium flows. He developed special "fluid wall" boundaries, designed to model moving isothermal walls. Soon afterward he, independently, developed homogeneous periodic ("Lees–Edwards") boundaries, in order to reduce the number-dependence of the viscosity [9]. Bill's fluid walls have just recently been reinvented, this time in Denmark [10].

Bill Ashurst and I continued our nonequilibrium simulations, reinventing Les Woodcock's velocity-scaling thermostatting method to go with both the fluid walls and the homogeneous flows. We needed contact with other researchers. Though the foreign travel budget at Livermore was mostly reserved for weaponeers, I was able to get permission to go to Paris, to visit with Hansen, Levesque, and Verlet. In 1977 I was allowed to spend a Fulbright leave in Australia. I made elaborate plans to work with Bob Watts on nonequilibrium viscosity simulations using his favorite water potential [11]. Bob's water potential turned out to be unstable, ending the project after about one week. Bob immediately became Director of the Research School of Chemistry's Computer Centre, again leaving my research unconstrained. At the Center my colleague across the hall was Bob's student, Denis "Bigfoot" Evans, who has ever since been one of the most enthusiastic and energetic contributors to the literature on nonequilibrium simulation. Most of my research in Australia was carried out with Denis and my son Nathan.

In view of the lack of useful theories far from equilibrium, we made an effort to establish links between our simulations and conventional classical mechanics. I first

described an adiabatic Hamiltonian basis for simulating periodic shears and compression at a meeting honoring Mel Green in April of 1979. Bob Zwanzig interrupted my talk with the disconcerting remark that my "new" approach was actually "well-known". At the conclusion of the meeting he and I went upstairs, to the library. I was surprised to find that (1) Zwanzig was again wrong and (2) that the National Bureau of Standards library was as empty on a 1979 evening as is the Livermore National Laboratory library on a typical 1996 one. In Sitges, the next summer, at another meeting honoring Mel Green, I again talked about the Hamiltonian basis for adiabatic deformation [12]. This time Zwanzig was the session chairman. He did not interrupt. By the time this work was published in Physical Review [13], Hans Andersen had discovered, independently, the same motion equations [14]. Around this same time, summer 1980, I had a major disappointment. I discovered that my marriage of 25 years had deteriorated. It came to an end in 1986. Both physics and physicists turned out to be very valuable in putting this disappointment behind me.

In 1984, Shuichi Nosé published a significant generalization of mechanics. He incorporated the ideal-gas temperature scale into time-reversible dynamical simulations in a way exactly consistent with Gibbs' statistical mechanics [15]. Within three years Brad Holian, Harald Posch, and I had established that Nosé's discovery links the macroscopic Second Law of Thermodynamics to time-reversible microscopic particle mechanics [16]. Just last year I was able to show that a special case of Nosé's mechanics follows from Hamilton's Principle [17]. Dettmann and Morriss have just found a Hamiltonian for this same special case [18]. So there is now an unbroken logical chain linking classical reversible mechanics to macroscopic irreversible thermodynamics and hydrodynamics.

I first met Shuichi at one of Carl Moser's CECAM workshops, in 1984. Ever since, I have worked hard to popularize the use of his ideas *away* from equilibrium. During my 1985 sabbatical in Vienna, planned as a collaboration with Karl Kratky, I also became acquainted with Harald Posch, and began a very pleasant and productive collaboration with him. Harald had a work station which could follow the chaotic $\{q, p, \zeta\}$ trajectories of an equilibrium thermostatted Nosé oscillator. After an all-night computer simulation, very detailed Poincaré sections of the trajectories were waiting on the screen of Harald's work station. They were then officially recorded by a photographer wearing a long white coat. So Harald and I became acquainted with Hamiltonian chaos together [19]. In early 1986, with Bill Moran, I found that the puzzling theoretically-established divergences of nonequilibrium phase-space densities were simply manifestations of the formation of multifractal phase-space distributions. This result, and its consequences, are still in the process of diffusing through the literature [20,21].

Nosé kindly invited me to spend the year 1989–1990 with him at the Hiyoshi campus of Keio University, in Yokohama. I accepted. In preparation for the trip, my son Nathan acquired the necessary credentials to perform a marriage ceremony for Carol and me. Brad Holian was my best man, just as I had been his a few years earlier. Besides furnishing a motivation to marry, the trip to Japan also looked like the perfect opportunity to find out more about time-reversible thermostats by working with the

man who had discovered them. But, for reasons I still cannot fathom, Shuichi and I were unable to find a joint project to work on. Left again without a plan, I mostly collaborated with Carol, her colleague, Toshio Kawai, also at Keio, Sigeo Ihara, at Hitachi's Kokobunji Research Center, and Tony De Groot, back in Livermore, on the simulation of plastic indentation. Our massively-parallel million-atom simulations [22,23] were the state of the art in 1990.

Every few years at the Livermore Laboratory I would get a new supervisor. Usually he would request, or at least hint, that I should occasionally do something "useful". Fortunately, this pressure to produce was reduced greatly, in my case, by the happy circumstance of my joint appointment in the College of Engineering at the University of California's Davis/Livermore campus. During most of my tenure in the Department of Applied Science, Fred Wooten, a true gentleman and a fine bridge player, was chair. In the Livermore Laboratory the useful work it was hoped that I would do was expected to involve "real data" for "real" materials, certainly in three dimensions rather than two, and preferably on a problem which had consistently frustrated able scientists and engineers for decades. My occasional attempts to help out resulted in work on plasticity, fracture, detonation, and the equation of state of hydrogen, none of which was particularly satisfying. The frustration stemming from the unwelcome but inevitable bureaucratic nudges toward "real applications", eased my recent decision to take a lucrative early retirement from the Livermore Laboratory, in mid-1995.

Aside from some successes with plasticity and indentation, my "applied" work was relatively unproductive, though my last formal defense of it brought forth unexpected fruit. Every year I had to make an appeal to a large committee of laboratory managers for the use of their scarce research funds. Toward the end of my 20 min I was asked by Tom Weaver, "Have you thought about using smooth particles?" I had never even heard of them. This chance question launched my research investigations for the past few years. I eventually located a smooth-particle expert, Larry Cloutman, only ten meters from my Livermore Laboratory office. He led me to the smooth-particle literature [24–26], and also generously lectured to my Department of Applied Science class on numerical methods. Since then, for four years now, I have been exploring, assimilating, and propagating smooth-particle lore with great enthusiasm.

Numerical continuum simulations using particles are an interesting and rewarding research area for several reasons. The programming is simple and transparent. The method is robust. The study of turbulence using smooth particles has particular interest. It presents an inverted version of Boltzmann's reversibility paradox, with macroscopic reversibility giving rise to microscopic irreversibility. Smooth particles also make it possible to study a variety of interesting macroscopic instabilities, quickly and cheaply. So far only a few detailed definitive comparisons with other techniques have been carried out. This is a consequence of the high stakes involved in numerical continuum simulation, a relatively contentious and competitive field. Despite this latter feature, I enjoy smooth-particle work so much that I have decided to devote the remainder of this talk/paper to some joint research carried out with Oyeon Kum, Harald Posch, and my wife Carol [27]. Harald Posch will describe some further smooth-particle results.

2. SPAM: Smooth-particle applied mechanics

After learning how to move particles, it is appealing to try to solve continuum problems in a similar way. Though the same kinds of constraint and driving forces used in molecular dynamics apply, the continuum problems seem to be simpler. This is because fluctuations are typically absent from continuum problems. On the other hand, the unstable nature of turbulent flow is really just a macroscopic manifestation of the Lyapunov instability familiar from atomistic simulations. This has become clear gradually through comparisons of the microscopic instability spectra [28] and transport coefficients [29,30] with their macroscopic turbulent analogs.

Smooth-particle applied mechanics solves the continuum equations for the time development of the coordinates, velocities, and specific energies $\{r, v, e\}$ of a moving grid of "smoothed" particles. The method includes an interpolation scheme for evaluating all the continuum variables, at every point in space, in terms of the discrete set of particle values. This specially stable particle method was discovered in 1977, by Lucy and by Monaghan [24,25], and has since been developed by astrophysicists and weapons physicists for a variety of fluid and solid applications [26]. This computational method is pedagogically appealing because it is simultaneously robust and simple. Typically, smooth-particle applied mechanics is implemented so as to conserve mass, momentum, and energy exactly. Angular momentum is not normally conserved. Though fixed boundaries can be easily modelled, moving boundaries and material interfaces require special consideration.

By eliminating an ordered grid, the smooth-particle method also eliminates the usual grid-based distortional instabilities which plague simulations with large deformations. Surprisingly, the particle picture simplifies the evaluation of gradients. Particles, rather than regular ordered grid points, also simplify automatic rezoning, interpolation, and the evaluation of fast Fourier transforms. The characteristic idea underlying the method is to describe the spatial influence of each particle through a relatively short-ranged "weight function" $w(r < h)$. Such a function is analogous to a pair potential. The weight function has at least two continuous derivatives so that the stress and heat-flux divergences $\{\nabla \cdot \sigma, \nabla \cdot Q\}$ vary smoothly in space. A typical smooth-particle weight function is Lucy's, here normalized for three-dimensional space:

$$w_{Lucy} = (105/16\pi h^3)[1 + 3(r/h)][1 - (r/h)]^3, \quad r < h .$$

At any point in space, r, the corresponding mass density ρ_r, including, as a special case, the density at the location of the ith smooth particle, ρ_i, is evaluated by superposing contributions from every particle within the range h of the point in question:

$$\rho_r = m \sum_j w_{rj}; \rho_i = m \sum_j w(r_{ij}) = m \sum_j w_{ij} .$$

In such pair sums, one for each particle, a typical smooth particle interacts with from 20 to 80 neighboring particles.

The smooth-particle form of the continuum equation of motion, $\rho\ddot{r} = \nabla \cdot \sigma$ illustrates the simplicity of the gradient operation using smooth particles. The divergence of the stress tensor becomes a sum of individual particle stress tensors weighted by the gradients of all the weights for particles close enough to interact:

$$\{\ddot{r}_i = m \sum [(\sigma/\rho^2)_i + (\sigma/\rho^2)_j] \cdot \nabla w_{ij}\} .$$

These simple motion equations lead to a surprising analog of Boltzmann's reversibility paradox [31]. They correspond exactly to atomistic Newtonian equations of motion if the hydrostatic stress tensor appropriate to a two-dimensional isentropic gas is used, $\sigma \propto \rho^2$. Though an atomistic SPAM system certainly has viscosities [29] and a conductivity [30], it is simultaneously a model for an isentropic gas which lacks these same transport coefficients. These phantom transport coefficients are an interesting paradox. That is, if the smooth-particle weight function $w(r)$, is viewed as a pair potential $\phi(r)$, the pair potential implies both shear and bulk viscosities – though the bulk viscosity must be nearly zero – and a heat conductivity, even though the isentropic gas being modelled has none of these properties.

Oyeon Kum, Harald Posch, and I devoted two years to the study of smooth-particle techniques, beginning with studies of linear shear flows and heat flows; then exploring more complex inviscid flows and the initiation of hydrodynamic instabilities [27,32]. All of our early work was restricted to two space dimensions. More recently, Carol and I have been carrying out three-dimensional studies. Oyeon, Harald, and I were able to obtain accurate solutions of a well-studied thermal convection problem, the "Rayleigh–Bénard problem", validating the smooth-particle solutions by comparing them to others obtained by applying conventional grid-based methods to the same problems [32].

Fig. 1 shows speed, temperature, and density surfaces for a typical stationary flow. Thermodynamically, the fluid is an ideal gas with a constant shear viscosity and a constant heat conductivity. The fluid is heated along the bottom wall of the container, expands, and is lifted upward. The buoyancy forces can generate either stationary or chaotic convection currents. Stationary solutions are rather well-known because they can be approximated by both grid-based and spectral techniques. Chaotic solutions are not so easy to validate. Numerical techniques can fail to converge. Even when they do converge, the chaotic solutions must be characterized through time averages. Politically-incorrect *two*-dimensional problems are not only much faster to solve and much simpler to observe. They also furnish valuable flow data for checking the more-cumbersome three-dimensional solutions of the type shown in Fig. 1. Oyeon, Harald, and I generated several two-dimensional solutions, emphasizing the ideal-gas and van der Waals equations of state.

We concentrated on a cell with a horizontal-to-vertical aspect ratio of two. This was because Chandrasekhar's classic approximate solutions for this case [33] suggested that two parallel rolls would result, as in Fig. 1. His analysis of this two-dimensional problem predicted the temperature difference leading to the onset of convection with an error of only a few percent. Later, in three-dimensional simulations carried out in Berlin and Livermore, there were some surprises. First, I found that the three-dimensional

Fig. 1. Surfaces of constant speed, temperature, and density according to two versions of Rayleigh–Bénard flow. At the left is a stationary grid-based solution of the

Navier–Stokes equations sometimes produced a solution with elliptical rolls, 30% narrower than in two dimensions, and rotated 45° from their expected orientation in the periodic cell. Soon afterward, another graduate student, Vic Castillo, discovered that a variety of stationary flows, with two rolls, four rolls, etc., can be generated in two-space dimensions [34]. Under some circumstances grid-based numerical solutions showed that two or more solutions can coexist with exactly the same boundary conditions, so that the observed solution is sensitive to the initial conditions.

Three-dimensional grid-based solutions converge, fairly convincingly, to stationary flows. Back at Livermore, with faster machines, Carol and I tried to simulate three-dimensional flows with smooth particles. Our early attempts failed, just as had Oyeon's in two dimensions, and for the same reason. The "fluid", rather than circulating, froze solid. The cause of the freezing can be readily understood. If the fluid flow velocity is too small to overcome the smooth particle potential barrier, which is of order h^{-D} in D dimensions, the flow stops. Making the barrier lower, by increasing h, leads quickly to simulations with millions of particle-pair interactions, impractical on serial machines.

The freezing and numerical diffusion associated with the smooth particles led to further studies, in Berlin, Livermore, and Vienna, of the intrinsic numerical viscosity and heat conductivity characterizing weak smooth potentials. Hess, Posch, and I [29,30] found that the additional momentum and heat flows caused by the discretization are closely analogous to the turbulent transfers of momentum and energy, reinforcing our prejudice [28] that turbulence and the many-body problem are one and the same.

In the course of comparing two- and three-dimensional simulations of the Rayleigh–Bénard problem, it was amusing to find that a three-dimensional fluid with no bulk viscosity

$$\sigma_{xx} = \sigma_{eq} + (\eta/3)(4\dot{\varepsilon}_{xx} - 2\dot{\varepsilon}_{yy} - 2\dot{\varepsilon}_{zz}) + 0(\dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy} + \dot{\varepsilon}_{zz}); \sigma_{xy} = \eta\dot{\varepsilon}_{xy} ,$$

does not correspond exactly to a two-dimensional fluid with only shear viscosity. To match the three-dimensional stresses, σ_{xx} and σ_{yy}, the two-dimensional fluid requires a bulk viscosity equal to one-third the shear viscosity, $\eta_v = \eta/3$:

$$\sigma_{xx} = \sigma_{eq} + \eta(\dot{\varepsilon}_{xx} - \dot{\varepsilon}_{yy}) + \eta_v(\dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy}); \sigma_{xy} = \eta\dot{\varepsilon}_{xy} .$$

The numerical effect of the additional bulk viscosity is typically quite small. In an ideal-gas simulation of Rayleigh–Bénard flow, at a Rayleigh number of 3600, the flow velocity increased by about on part in 1000 when the two-dimensional bulk viscosity was set equal to zero rather than to $\eta/3$.

We are continuing the Rayleigh–Bénard work, and undertaking analyses of smooth-particle shockwave structure, on the massively-parallel computers at Livermore, testing the stabilities and size-dependence of corresponding two-dimensional and three-dimensional simulations. Evaluating the promise of smooth particles, relative to more conventional methods, is good research: deeply absorbing, technically challenging, sometimes surprising, and possibly even useful. I am very grateful to my many friends and colleagues for helping to make these studies a reality.

3. Summary

I appreciate the trouble which Brad Holian and Michel Mareschal went to in organizing this meeting in Lyon. Ever since Jean-Pierre Hansen introduced me to Paris, international gatherings, particularly the CECAM workshops and NATO institutes, have been invaluable sources of stimulation for my research. Nonequilibrium simulations at the atomic level, though no more "realistic" than Boltzmann's kinetic theory, have an aesthetic unity, appeal, and value. I particularly appreciate the honor that Brad and Michel have done me here, and am looking forward to seeing continuing progress in nonequilibrium simulations, both microscopic and macroscopic.

Addendum of 20 July 1996

A cancelled weekend with Jean-Pierre left Carol and me at CECAM, with plenty of time to digest the mixed food-for-thought provided by our friends, old and new. Sauro Succi suggested some novel ways to link SPAM with traditional statistical theories. One of the nicest birthday presents emerged from my conversations with Carl Dettmann. He provided the elusive answer to a puzzling question which came up in 1984: What is the simplest Lagrange–Hamilton basis for Nosé–Hoover mechanics? Carl found the answer quickly: Nosé's original Hamiltonian, multiplied by s. No time scaling is required. The only trick is setting the initial value of the Hamiltonian equal to zero. This result leaves Gibbs' ensembles firmly linked to a mechanics so classical that even Goldstein would have recognized it. From my perspective, nonequilibrium statistical mechanics has finally reached the maturity of its equilibrium cousin, and just 25 years later. Now, the basic principles linking transport and the Second Law to mechanics, fractals, and Lyapunov instability are an enduring part of physics. Both the computational and the theoretical workers have their own routes to understanding, and are now at work on the details. It is promising for the future to see that both groups are hard at work on representing boundaries, stimulated by the work Lyderic Bocquet described. Both Berni and Alex Garcia rightly emphasized the importance and the promise of hybrids to linking the microscopic and macroscopic points of view. Harald, Carol, and I like SPAM. I personally profited from the chance to talk with Michel and Malek Mansour about their experiences with the degenerate instabilities they found in Rayleigh–Bénard problems. My own student, Vic Castillo, has been rediscovering very similar degeneracies at Livermore. Pierre Gaspard is blazing his own Hamiltonian path to nonlinear transport while a host of simulators continue their comprehensive explorations of this relatively new territory. For me, the tantalizing goal has again shifted, from equilibrium, to nonequilibrium, to understanding instability and turbulence through SPAM. The continuing search sometimes leads to sweeping views of the future. The beautiful view from Lyon guarantees excitement and stimulation for the birthdays yet to come. Thanks again, Michel and Brad, for making it possible to meet the many friends assembled here at Lyon.

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