50 Years of Computer Simulation — a Personal View

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Abstract

In the half century since the 1950s computer simulation has transformed our understanding of physics. The rare, expensive, slow, and bulky mainframes of World War II have given way to today's millions of cheap, fast, desksized workstations and personal computers. As a result of these changes, the theoretical formal view of physics has gradually shifted, so as to focus on the pragmatic and useful. General but vague approaches are being superceded by specific results for definite models. During this evolving change of emphasis I learned, developed, and described my simulation skills at Michigan, at Duke, at Livermore, and in Nevada, while forming increasingly wide-ranging contacts around the world. Computation is now pervasive in all the scientific fields. My own focus has been on the physics of *particle* simulations, mainly away from equilibrium. I outline my particle work here. It has led me to a model-based understanding of both equilibrium and nonequilibrium physics. There are still some gaps. There is still much to do.

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I. INTRODUCTION

Computer-induced changes in emphasis have transformed what it means to "understand" physics. This transformation is nowhere more striking than in the many-body model-based subjects of statistical mechanics and kinetic theory. The *old* way was solving many-body problems "in principle" (but not "in fact"), by formal expansions around the ideal gas or the harmonic crystal. The *new* way has replaced the expansions with direct numerical simulations of model systems. At equilibrium, ensemble-based "Monte Carlo" simulations are appropriate. "Molecular dynamics" simulations are more generally useful because they apply to both equilibrium and *nonequilibrium* situations. The nonequilibrium problems typically involve flow and gradients and are quite unlike their static homogeneous equilibrium relatives. Writing down the governing equations for a many-body model (a sum over states, or the dynamical equations of motion, for instance) is now considered just a beginning challenge, not an end in itself.

Masaharu Isobe thought my reminiscences would interest younger readers of this Journal, "Ensemble". Besides the name's possible link to Gibbs' ensembles, the name "Ensemble" also suggests cooperation, and "working together". These are nice concepts, which underlie the steady progress of science, particularly in today's electronic world, with the immediacy of the internet and email making efficient timely international collaborations possible.

I agreed with Masaharu's idea, and summarize some milestones of my work here. Though times and tastes change, the experiences of learning, creating, and teaching trace an enduring continuity worth considering and summarizing. Here is a bit of my own simulation history, with the hope it will prove useful to yours. I start out with my college and university days in Ohio and Michigan, and end up with retirement in Nevada. Many more details can be found on my website [http://williamhoover.info].

II. OHIO, 1953-1958, AND MICHIGAN, 1958-1961

My small and isolated undergraduate college, Oberlin College in Ohio, featured and encouraged the sceptical attitude so useful in physics. Otherwise the scientific content of my Oberlin liberal-arts coursework was irrelevant to my research career. The classroom instruction in mathematics and physics was formal, and mired in the past. This disap-

pointing style of instruction very nearly convinced me to switch from science to economics, my Father's field of study.

Recuperation from an automobile accident kept me out of college for a semester. I attended Harvard's Summer School to make up the Physical Chemistry course I had missed. The lecturer, Stuart Rice, provided research excitement and strengthened my commitment to science. Stuart loved kinetic theory. He reassured us students that any shortcomings in the practical labwork portion of his course would have no influence on our grades.

My graduate university, the University of Michigan in Ann Arbor, was a great improvement over Oberlin. The University of Michigan provided useful coursework, state-of-the-art computational tools, as well as the stimulation and inspiration necessary to research. Shortly after my arrival there I came upon Alder and Wainwright's "Molecules in Motion" article in Scientific American[1]. The so-different pictures of hard-sphere fluid and solid trajectories in that article are still worth a look today. See **Figure 1** for a pair of example pictures taken from Farid Abraham's 1980 work on the melting transition[2]. In the 1950s, simulating the motion of 108 particles was a challenge. The Alder-Wainwright pictures triggered my interests in microstructure and molecular dynamics.

At Michigan, Andrew Gabriel De Rocco, a young Chemical Physics Professor and my PhD thesis advisor, was excited by statistical mechanics. He had a rare knack for relating formalism to the real world. What constitutes the "real world" is of course a matter of opinion. I well remember Andy's wife Sue, who overheard one of our upstairs conversations on pair potentials, shouting up the stairs: "Andrew, *all* your potentials are repulsive!" Tastes differ!

As a result of Andy's enthusiasm and support I became an expert in the Mayers' "virial" expansion, the expression of fluid pressure as a power series in the density. B_n, the nth coefficient in the series is a sum of relatively-complicated n-body integrals. The integrands of these integrals are products of as many as $n(n-1)/2$ functions linking the n particles together. For hard parallel squares and cubes these integrals can be done analytically[3], though beyond B_6, the topological bookkeeping requires a fast computer. By 1960 I had the patience and the training to program the FORTRAN calculation of a few million of these integrals, using the "MAD" computer [Michigan Algorithmic Decoder][4]. Programming was then a bit tedious. It involved writing instructions in the form of punched cards, one card for each program line. But it had to be done. For

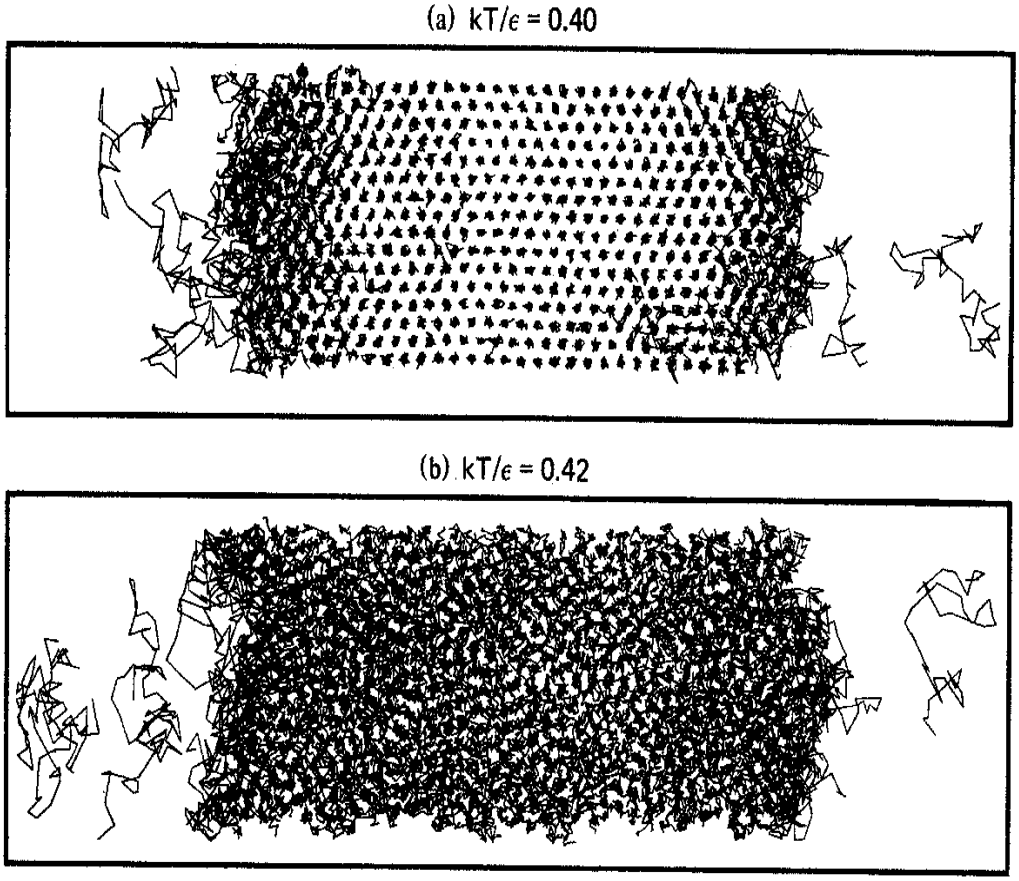

Figure 1: Atomistic trajectories just below (top) and just above (bottom) the melting temperature, taken from Reference 2.

parallel cubes B_7 required computing $468 \times 7! = 2,358,720$ separate integrals! MAD made occasional irreproducible machine errors. These errors were useful reminders of the need for vigilance in numerical work. The violation of obvious requirements (such as conservation of momentum and energy) is the usual result of logical or typographical errors in programming.

Once the program was successfully punched out, and carefully checked, I found *negative* virial coefficients, both B_6 and B_7, for hard *repulsive* parallel cubes. Negative tensile contributions for positively repulsive particles was a big surprise! I was thoroughly hooked by the excitement of research. Of course the pace was slower then. I exchanged several letters with "H. N. V." Temperley about the details of the virial series. After a few letters the "H. N. V." changed to an informal "Neville". A typical US $\leftrightarrow$ UK roundtrip correspondence took two weeks by airmail. Bob Zwanzig had published the paper[3] which introduced me to hard cubes but which also wrongly contradicted my negative-coefficient

results. It was a real thrill, and a lesson, when, in a phone conversation with Andy and me, he readily admitted his mistake.

III. DUKE UNIVERSITY, DURHAM, NORTH CAROLINA, 1961-1962

In the 1960s in America a postdoctoral appointment was required before seeking out a "real job". Andy sent me on to Duke University, where one of John Kirkwood's students, Jacques Poirier, lived an isolated existence as a Professor of Chemistry with theoretical inclinations. The smell of menthol from the Salem cigarette plant traveled miles in the evening to our house on a dirt road next to a turnip field. The various organic smells during the day at the Chemistry Department helped make this a tranquil detour from mainstream physics. Because Jacques' ideas for our joint research turned out to be invalid I was able to pursue further work on the virial series while at Duke. In those days, when computer simulation was still rare, approximate integral equations for the distribution of particle pairs $g(r)$ were all the rage. Because the equations were nonlinear in $g(r)$, complete solutions required elaborate computation. But substituting a density expansion of $g(r)$, and equating coeffients of powers of the density made it possible to compute the approximate virial coefficients and compare them to the Mayers' exact expressions[5].

During the Duke year, I got in contact with George Stell, another *afficianado* of the Mayers' series, a skilled jazz musician, and still a great friend. I visited George in his Greenwich Village apartment. Two memories of that visit stand out: George had his own sauna there, and the relative calm in his apartment was broken by a sewergas explosion just outside, strong enough to levitate a heavy manhole cover. Once back at Duke I managed to land job interviews at the Livermore and Los Alamos Laboratories, the two rival computing giants overseen by the University of California. Alder and Wood, at the two laboratories where I would soon seek a job, were rivals too, disagreeing over their relative priority and contributions to the understanding of the hard-disk and hard-sphere melting transitions[6,7].

IV. LIVERMORE AND DAVIS, CALIFORNIA, 1962-2004

I interviewed at both Los Alamos and Livermore in 1962, flying out from Michigan to talk to a dozen or so scientists at each laboratory and giving a seminar on my virial-

series work. Los Alamos, in the mountains of New Mexico, was physically the more interesting of the two bomb laboratories. Livermore was located in a once rural grape and cattle ranching valley suffering now from pollution and urban sprawl. By the time I arrived Alder and Wainwright were studying disk and sphere systems of about 1000 particles, using both rigid and periodic boundary conditions. One of their research goals was understanding whether or not disks and spheres could freeze and melt at high density. My hard-particle virial series expertise fitted in well with that work[8].

At Los Alamos the relative humidity was low and the scientists wore Hawaiian shirts and desert boots rather than the suits of the Midwest. The salaries there were nearly 20 percent lower (partly a function of the longer five-week vacations due to the laboratory's remoteness). This difference in salaries decided me on Livermore, where Berni Alder provided me a home in the Physics Department. It was an exciting time and place. Particle, continuum, plasma, astrophysical and nuclear physicists all joined together, with weekly scientific meetings under Edward Teller's watchful eyes. For one of the talks Francis Ree and I got Teller's permission to pursue and present a computationally demanding single-occupancy explanation of the hard-disk and hard-sphere phase transitions[9]. Francis Ree, trained by Henry Eyring, was, like me, dedicated to precise and careful statistical analyses. We solved Berni Alder and Bill Wood's hard-sphere and hard-disk problems using both the Mayers' virial series (for the fluid phases) and Metropolis-Rosenbluth-Teller Monte Carlo simulations (for Kirkwood's single-occupancy solid phases). See **Figure 2**. Our "Monday Morning Meeting" presentation went well.

This Monday-Morning-Meeting background in a variety of disciplines was extremely useful to me later on, both scientifically and socially. Teller started the Department of Applied Science at Livermore in 1963, with the idea that a wide background (nuclear, quantum, classical, mathematical, chemical, electromagnetic) was essential to training students. I taught in the Department for about thirty years, and enjoyed it thoroughly. My wife Carol was a student in one of the statistical mechanics courses I taught at DAS.

The bookkeeping associated with hard-particle collisions made molecular dynamics seem less interesting to me (or at least harder) than Monte Carlo simulation. But in the early 1960s Rahman, Verlet, and Vineyard[10] all followed Fermi's 1950s work, in showing how to carry out simulations with continuous force laws. My group leader at the time, Russ Duff, supported my interest in learning molecular dynamics. As a shockwave experimentalist he liked the idea of simulating shockwave-induced melting with molecular

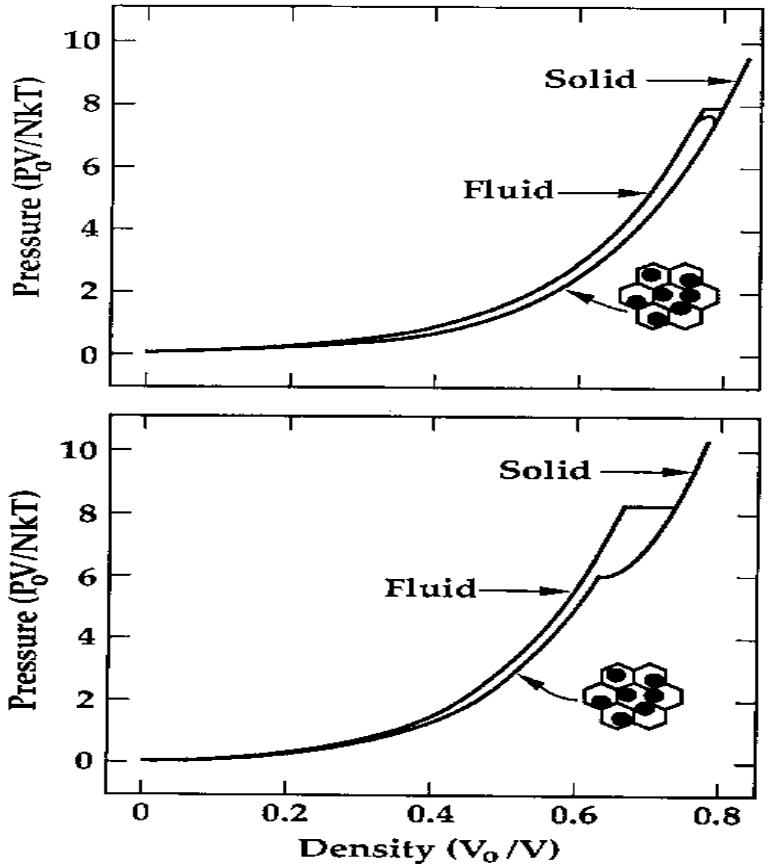

Figure 2: Hard-disk (above) and hard-sphere (below) equations of state. From Reference 9. The close-packed volume (area in two dimensions) is V_0. The lower "single-occupancy" curves correspond to the pressure of particles confined to space-filling cells, as shown in the insets.

dynamics. I took on the project, storing thousands of long particle trajectories on magnetic tapes. The physical stretching of some of these tapes made them unreadable often enough that the storage procedure was useless for long runs. The shockwave simulations of 1967 had to be put aside temporarily, and were not resurrected until 1980[11], when magnetic tapes were obsolete, and again in 1997[12], when the anisotropicity of temperature had caught my interest. **Figure 3** illustrates that interesting result from the shockwave work: in strong shockwaves temperature becomes a tensor. The longitudinal temperature (the velocity fluctuation in the direction of the motion) greatly exceeds the transverse temperature in strong shocks.

A later group leader of mine, Mark Wilkins, strongly influenced my scientific outlook. Mark was a self-taught expert in the numerical solution of the partial differential equations of continuum mechanics, specializing in plastic flow and fracture, essential for weapons

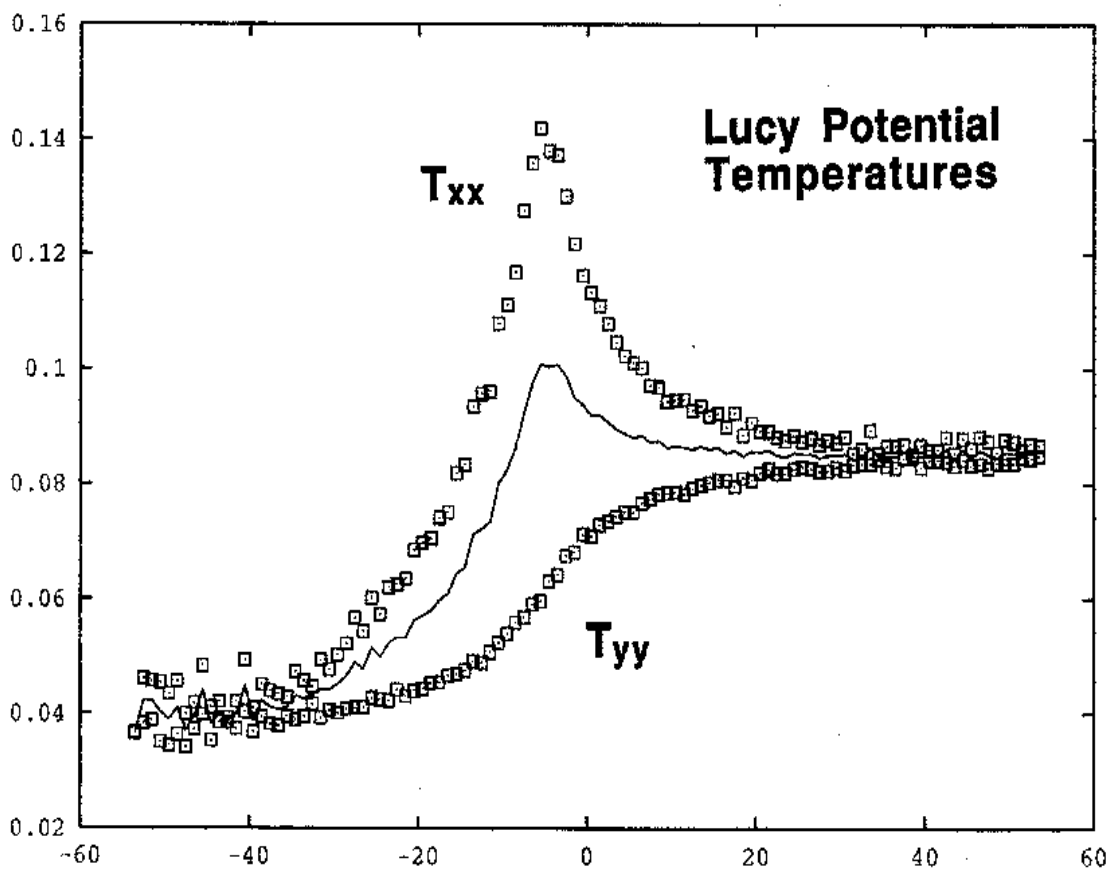

Figure 3: Longitudinal (top), mean, and transverse (bottom) kinetic temperatures in a Lucy fluid shockwave, taken from Reference 12.

simulations. Mark stressed that physics is a study of "models", closed sets of differential equations which bear some resemblance to our experiences in "real life". Quantum mechanics is such a model, and evidently quite imperfect, in that it never predicts the unique outcomes observed in the real world.

At the Livermore Laboratory of the 1960s there were plenty of interesting collaborators with whom I could work. Al Holt was a formalist, a tensor specialist who had been trained by chaos guru Joe Ford at Georgia Tech. Al's interest in elastic constants combined nicely with my own statistical and lattice dynamical skills. Dave Squire worked for the Army Research Office in Durham, North Carolina. He was a practical chemist, schooled by Zevi Salsburg, a colleague of Berni's. Dave was able to visit the Livermore Laboratory for several months in the late 1960s, along with his wife and eight children. Al and Dave and I formulated the elastic response of crystals to strain under both isothermal[13] and adiabatic[14] conditions. These results, which can be evaluated by either Monte Carlo or

molecular dynamics simulations, have been rediscovered frequently.

I visited the nearby IBM Research Laboratory at Almaden, which had managed to hire John Barker and Doug Henderson. I was invited there for a seminar and prepared a set of slides. Barker ran the slide projector while Henderson asked an occasional question. That was the whole audience at Almaden. I was fortunate, at Livermore, that dozens of scientists were actively doing research in statistical mechanics. In the late 1960s Barker and Henderson, along with Mansoori, Canfield, Weeks, Chandler, Andersen, Rasaiah, and Stell, developed a very successful perturbation theory for the Helmholtz free energy[15]. Only the hard-sphere pair distribution function was needed, and a useful form for that was available from the integral-equation work. The theory was actually useful for realworld equilibrium thermodynamic calculations. This equilibrium breakthrough convinced me it was high time to switch to the study of *nonequilibrium* problems, where the only theory available was Green and Kubo's linear-response theory of transport[16].

The energy crunch in the Carter administration led to mass firings at the Livermore Laboratory and to a change of emphasis and structure: suddenly there were lots of group leaders, lots of progress reports and proposals, and detailed budgets. When I needed dozens of hours of CRAY computer time to study the effect of Coriolis' forces on the heat flux, Roger Minich, a favorite of one of the bomb divisions, generously gave me the time from his weapons-physics accounts[17].

The cutback in basic research at Livermore made it necessary to look outside the laboratory for collaborators. I had a lot of fun working with Brad Holian at Los Alamos. We had a common interest in statistical mechanics and simulation. Brad tried to get a job at Livermore; I tried to get a job at Los Alamos, so that we could work together, but both these initiatives were unsuccessful.

In my attempts to satisfy the mounting laboratory pressure for "relevance" I carried out some dynamic fracture simulations with Bill Ashurst[18] and, in his PhD thesis work, Bill Moran. **Figure 4** shows a typical fracture specimen. At a meeting with the Laboratory Director, Mike May, Mike asked me whether or not these fracture simulations were really relevant. I had to admit that atomistic models are actually quite limited in scope, and are often misleading (even today).

Bill Ashurst, my first PhD student at the Department of Applied Science, was keen to simulate nonequilibrium flows. We developed methods for simulating shear flows with isothermal boundaries as well as periodic homogeneous algorithms[19]. Bill was able to

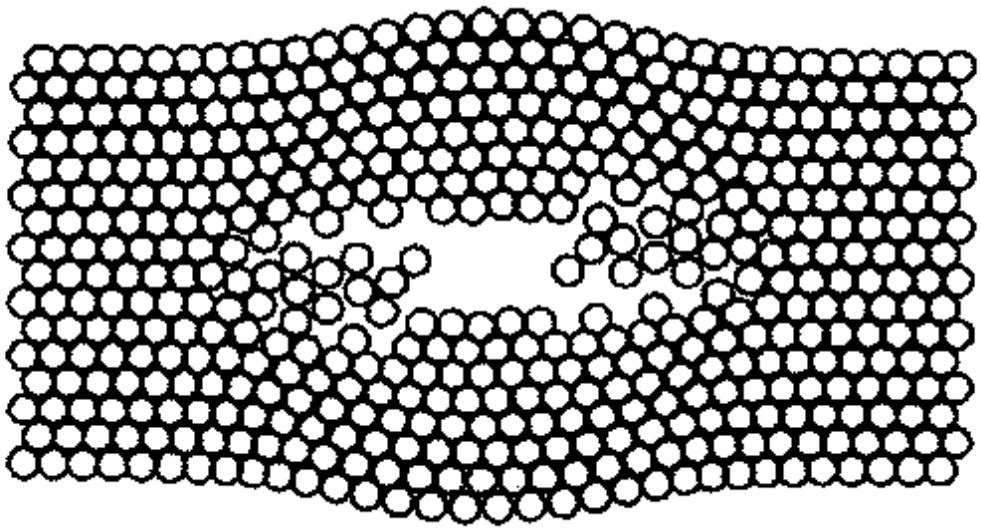

Figure 4: Fracture specimen simulation, taken from Reference 18.

make movies (as was also Brad Holian at Los Alamos). These movies were a fixture of small topical physics meetings in the early days of nonequilibrium molecular dynamics.

An early experience with the National Science Foundation was educational and helped sharpen my scepticism for government's ability to select good problems to solve. In the early 1980s I proposed a Fourier analysis of simple nonequilibrium distribution functions. The proposal was evaluated "excellent" by five reviewers and "very good" by the sixth. Despite this, the proposal was declined. This early failure reinforced my natural inclination to forgo begging for research funds.

V. TRAVEL, WITH SABBATICALS IN AUSTRALIA, AUSTRIA, AND JAPAN

After a first visit to France to confront Verlet, Levesque, and Kürkijarvi's somewhat erroneous Green-Kubo transport results[20] with the nonequilibrium analogs I had calculated with Bill Ashurst, Orsay became a regular stop for me. Carl Moser supervised a long series of workshops, seminars, and meetings, at CECAM (The European Center for Atomic and Molecular Simulation) which were seminal and stimulating. The locale, about an hour outside Paris in the countryside, was conducive to good work. There was a hillside covered with wild blackberries on the way to lunch and the Parisian bistros and restaurants attracted us in the evenings after work.

The Department of Applied Science and the Livermore Laboratory provided my financial support throughout each year. Though my salary was set by the Department, based on academic criteria, the Laboratory always tried to exert pressure toward "practical applications" to justify its paying the Lion's Share (five eighths) of my salary. As compensation for this pressure the "Professional Research and Teaching Leaves" available at the Laboratory made it possible to get away for sabbatical research. Such leaves, augmented by support from the Fulbright Foundation, Universität Wien, and the Japan Society for the Promotion of Science, took me and my family to Australia in 1977, to Austria in 1984, and to Japan in 1989.

In 1980, between my Australian and Austrian sabbaticals, I noticed that a Hamiltonian could be constructed which reproduced exactly the geometry and energy balance for a many-body system undergoing periodic shear. This was the "Doll's Tensor" Hamiltonian, which I described in June 1980 at Sitges[21] (Spain) after the StatPhys organizers for the August 1980 Edmonton meeting turned down my proposal to speak about it in Canada. "Doll's Tensor" was simply the tensor qp array, constructed of the Cartesian particle coordinates $\{q\}$ and momenta $\{p\}$. Adding the term $\dot{\epsilon}\sum yp_x$ to the usual many-body Hamiltonian induces a macroscopic motion with $\langle \dot{x} \rangle = \dot{\epsilon} y$, simple shear, or "Plane Couette flow". In June 1982, at Howard Hanley's seminal meeting, "Nonlinear Fluid Behavior", which I helped organize, I was finally able to present a talk on nonequilibrium molecular dynamics to a large mostly-American audience of interested colleagues[22].

By 1984 my desire to present the Doll's-tensor work as a talk at an international conference, the 1983 Edinburgh StatPhys meeting, had once again been frustrated. The consolation prize, a humorous poster detailing the history of the shear flow work, was not published until nine years later in the proceedings of a Sardinia meeting[23]. In reaction to all the StatPhys frustration, I organized, with Giovanni Ciccotti, a highly-successful Enrico Fermi Summer School meeting at Lake Como, where the new nonequilibrium algorithms were thoroughly discussed[24]. See particularly Denis Evans' lecture "Nonequilibrium Molecular Dynamics", pages 221-240 of the School's Proceedings.

Only very recently[25], with my wife Carol and Janka Petravic, I have quantified the errors (nonlinear in the strainrate $\dot{\epsilon}$) incurred by using the Doll's and the closely related S'llod algorithms. The kewpie doll has a highly-interesting history (the Centennial of the Doll is 2009!) in addition to its usefulness as a mascot for statistical physics.

With the shearflow problem solved, Denis Evans and Mike Gillan, working completely

independently, found an external field that correctly generated heat flow in 1982 – see again Evans' lecture[24] for the details. Their solution of this problem was particularly interesting because it provided a concrete example in which Gauss' Principle (equivalent to Least Action for equilibrium systems) gives incorrect motion equations (inconsistent with Green-Kubo) away from equilibrium[26].

The Australian Sabbatical experience had been interesting, though slightly chaotic. My proposed work at the Australian National University's Computer Centre, in Canberra, with Bob Watts, came to an abrupt end in the first week when Bob was appointed to replace the Director of the center. Watts' water potential, which I had intended to investigate in Australia, turned out to be unstable, making it possible to concentrate on what was for me a more interesting project, the determination of liquid and solid free volumes. My son Nathan, having just finished high school, was in Australia with me and we worked together at the ANU Computer Centre. That work involved a "gedanken experiment" in which a single very light particle traced out a "free volume" while its heavier neighbors stayed put[27]. I had used this same idea earlier to rationalize the use of cell models[28]. **Figure 5** illustrates the difference between the fluid and solid phases from this perspective. It was educational to learn from these results that the free volume in the fluid phase is actually smaller than that in the coexisting solid!

My first Austrian experience also had an unexpected turn. Rather than working exclusively with Karl Kratky, as I had intended, I began to collaborate with Harald Posch[28], whose interests in statistical mechanics and nonequilibrium simulations were similar to mine. Both Harald and I valued reproducibility and precision very highly. We often compared results from our two independently-written computer programs. Kratky was a formalist, and I soon lost patience waiting the months it took him to reproduce results I could generate numerically in a matter of days. The Austrian sabbatical gave me background for my first book, "Molecular Dynamics", lectures given at Universität Wien and written up once I was back at Livermore, in 1986. In those electronically primative times it was necessary to edit the teX file for the manuscript in one building and to drive about a half mile to another building to see a printout. Because car travel was limited until 18:00 during the week, most of the book work had to be done at night.

Prior to a 1984 CECAM workshop at Orsay I had the very good fortune to meet Shuichi Nosé on the Orly Airport train platform. (I had noticed his surname printed on his suitcase.) This meeting eventually led to a very pleasant and creative year in Japan.

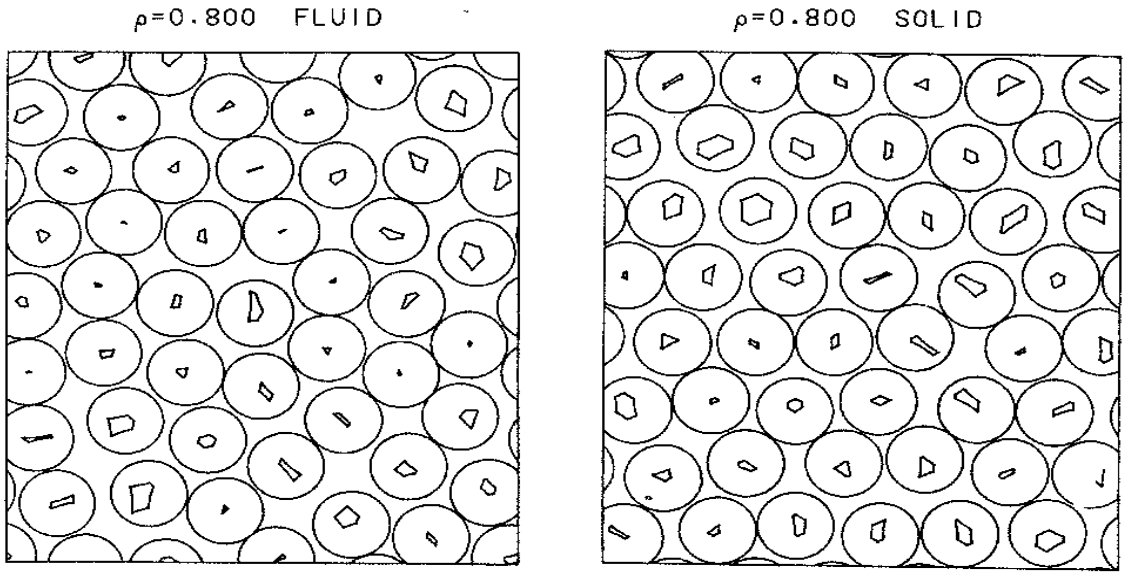

Figure 5: Fluid (left) and solid (right) hard-disk free volumes at a common density four-fifths of close packing. The "free volumes" shown are the regions available to the center of each disk when the remaining disks are held fixed. Taken from Reference 27.

Nosé was isolated from the other workshop members, choosing to stay in a Japanese-style hotel. We arranged to meet at the Notre Dame cathedral. On a bench in front of the church we talked about his novel thermostat ideas[30,31] in detail. After the workshop I visited Philippe Choquard in Lausanne to work out the consequences for a harmonic oscillator. The result was my most cited paper[32]. Some of the oscillator orbits were quite beautiful[33]. **Figure 6** shows a regular periodic orbit for a thermostated oscillator. The oscillator exhibits chaotic orbits too. "Chaotic" orbits have the property of Lyapunov instability – an infinitesimal perturbation of such an orbit grows exponentially fast with time. Orbits for dissipative systems, in which work is converted to heat, are typically "fractal" with a fractional dimensionality less than that of the space in which they are embedded. See **Figure 7** for an example.

My interest in computational thermostats was immediate and has continued to this day. I asked Berni Alder what he thought about my energy and temperature-control ideas. He pooh-poohed the notion. I traveled to Los Alamos to ask Bill Wood for his ideas. Though a bit more diplomatic, his thoughts were the same as Berni's: thermostats were not a very useful idea. Fortunately, I had the freedom to spend much of the next few years working out the details, linking thermostats to statistical physics. Bill Moran

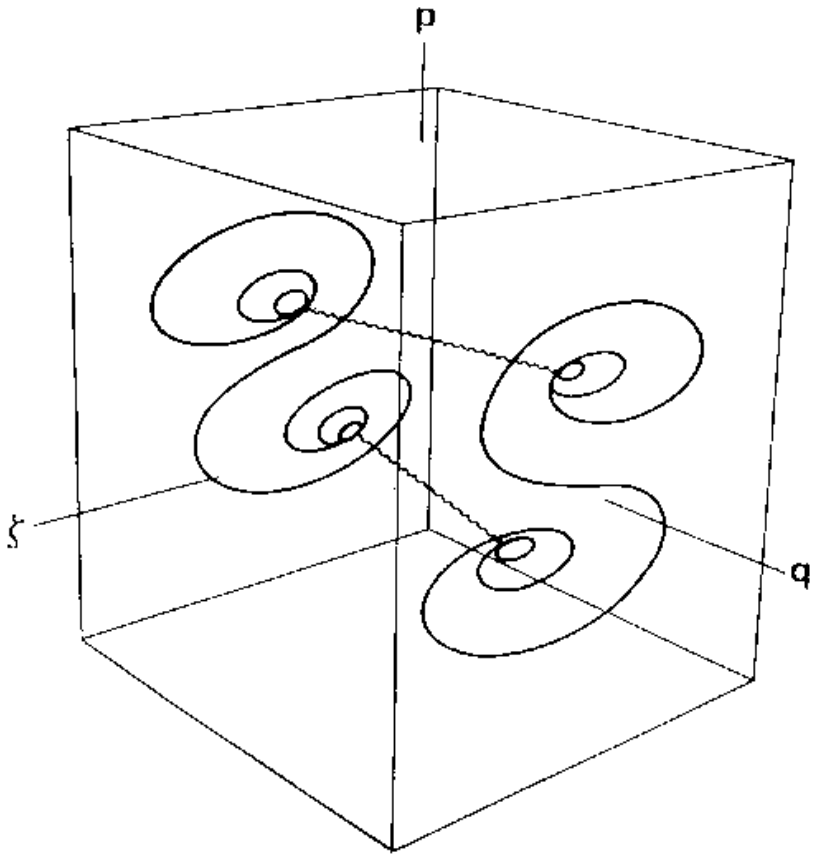

Figure 6: Periodic orbit for a thermostated harmonic oscillator with coordinate q, momentum p, and friction coefficient ζ, taken from Reference 33.

and I generated the fractal objects which describe the collisions taking place for a very simple problem. We studied a thermostated particle falling through a periodic "Galton Board" of hard-disk scatterers[34]. The collisions formed a multifractal object, with the dimensionality of the object decreasing with increasing field strength. For a sample see **Figure 7**.

The finding that the dimensionality of phase-space distributions was reduced below that of Gibbs' equilibrium distribution was a revealing and rewarding insight for me. The extreme rarity of the fractal nonequilibrium states explained irreversibility. Because the equations of motion are time-reversible and the probability of choosing an initial fractal state is of measure zero, the probability of *violating* the Second Law of Thermodynamics, along a time-reversed trajectory, vanishes. The fractal nature of the phase-space distributions also showed that there could be no nonequilibrium entropy. This is because Gibbs' recipe for the entropy in terms of the N-body distribution function f and Boltzmann's

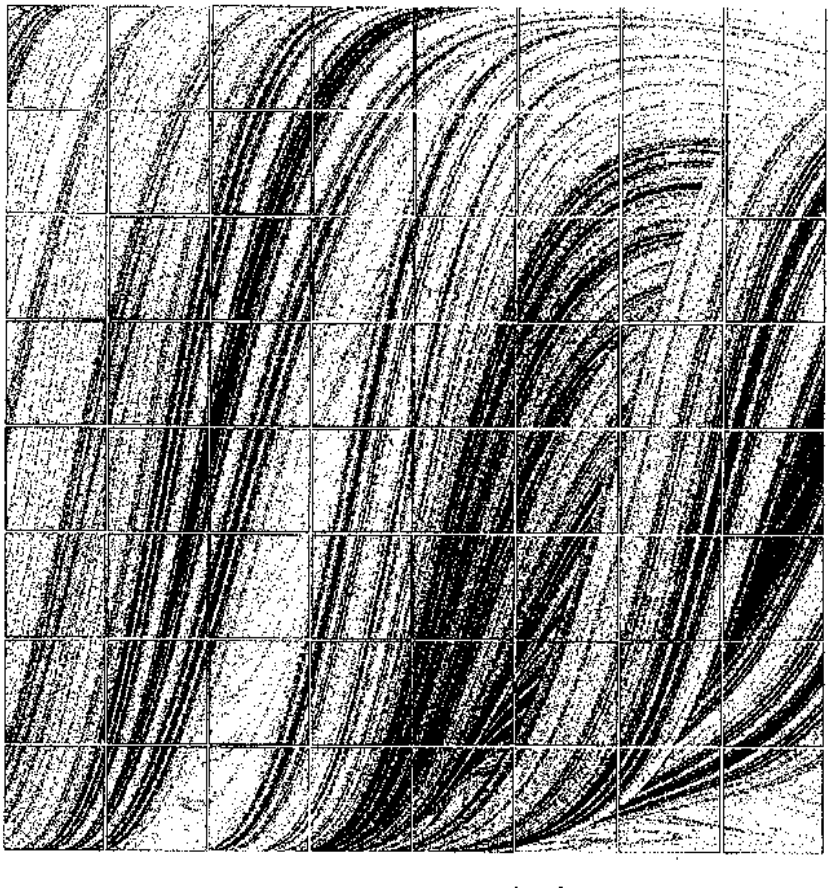

Figure 7: A multifractal phase-space plot of successive collisions in the Galton Board problem with a constant vertical gravitational field. The abscissa corresponds to the location of each collision on a hard disk scatterer from bottom (at the left) to top (at the right) relative to the downward field direction. The ordinate corresponds to the tangential velocity component, which varies from -1 (at the bottom) to $+1$ (at the top). The motion of the moving particle is constrained to a constant speed of unity, as explained in Reference 34.

constant k,

$$S_{\rm Gibbs} \equiv -k\langle f \ln f \rangle \ ,$$

diverges when f is singular.

At the New York American Physical Society meeting emphasizing the hot topic of "High-Temperature Superconductors" I took long walks in Central Park, mentally estimating the phase-space dimensionality loss in strong shockwaves and ruminating over the paradox that time-reversible equations of motion lead to irreversible behavior. Much later these topics gave rise to my third book, "Time Reversibility, Computer Simulation,

and Chaos". Oddly enough, much of today's research still deals with equilibrium problems, though to me nonequilibrium ones are more numerous, more significant, and more interesting.

In the years following my 1977-1978 sabbatical Down Under, nonequilibrium molecular dynamics had been developing rapidly. In this same period, my marriage was deteriorating. The years from 1980 through my divorce, in 1986, were particularly difficult, but still relatively productive. In 1988 a very lucky chance meeting with a visitor to the Livermore laboratory, a young researcher from Louisiana State University, a Doctor Gupta, brought me in contact with his host, a former student of mine, Carol Griswold Tull. Carol was working with the Livermore supercomputers and her own marriage had ended in 1984. We were fortunate to share very similar interests in a "Good Life" mixture of science, nature, music, and nourishment. At last I had found a faithful woman with whom to share my life. Our marriage was arranged for 1989, so that we would arrive for our sabbatical in Japan as an officially married couple. My son Nathan performed the ceremony in Carol's Livermore home.

The Japanese experience, at Keio University in Yokohama, was a surprise. After finding that there seemed to be no plan to collaborate with Nosé, who had invited me to visit Keio, I prepared a list of about a dozen projects on which we might work together, and took it to his office for discussion. Still nothing. In retrospect this turned out well, at least for me, in that it freed up my time to write another book, "Computational Statistical Mechanics", summarizing what I had learned in my Applied Science teaching at Livermore while enjoying the peaceful work atmosphere of Japan. Carol and I spent many a night at the computer laboratory near Hiyoshi station, working on the manuscript. Our Hershey House apartment, overlooking a busy baseball field was within walking distance so that our working hours weren't limited by the train schedules.

At Hershey House we got weekly progress phonecalls from Tony DeGroot, back in Livermore, who had built a 64-processor parallel computer capable of million-atom molecular dynamics. Working with Tony and Jeff Kallman in Livermore, with the support of Irv Stowers and Fred Wooten, as well as collaborating with Taisuke Boku, Toshio Kawai, and Sigeo Ihara in Japan, we worked long-distance on color movies of silicon crystal deformation. A still picture from such a movie is shown here in **Figure 8**. This collaboration, with nine coauthors, involved the work of more individuals than did any other of my research efforts[35].

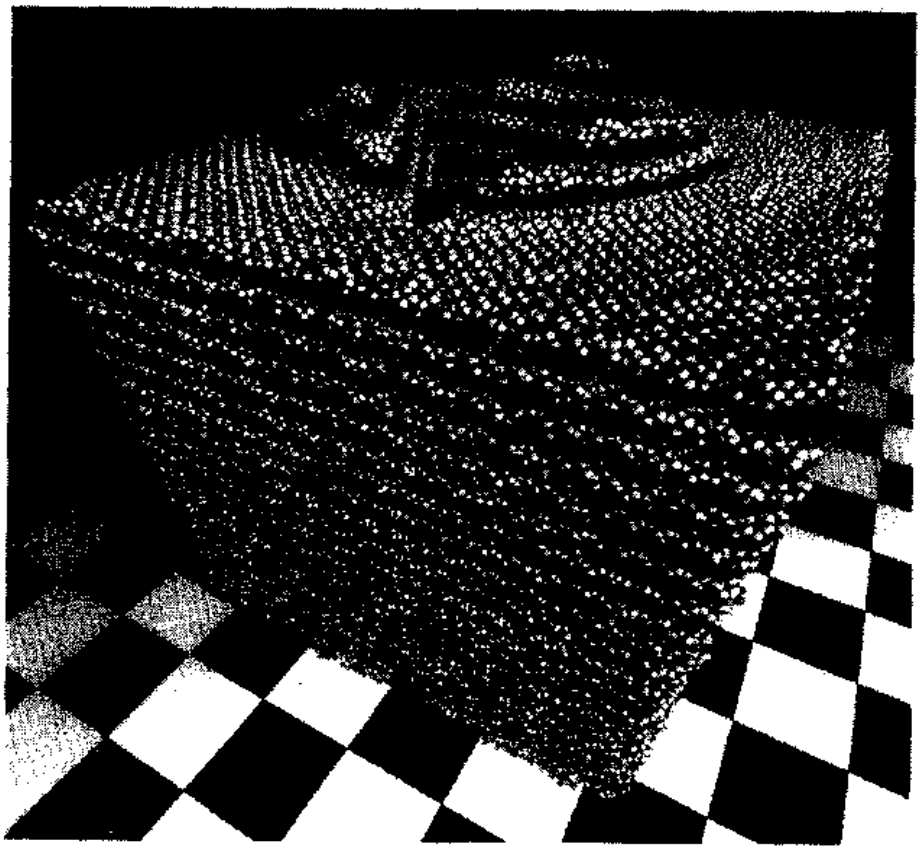

Figure 8: A plastic indentation pit in a 373,248-atom model of silicon. The indentor (not shown) is tetrahedral in shape and moves at one-fifth the sound velocity. Analogous two-dimensional indentation simulations are described in Reference 35.

After the Berlin Wall came down in 1989 the Livermore Laboratory was left without a mission, and became a vestige of its former self, doing "work for others" and striving to appear practical. In this climate Teller's Department of Applied Science lost its appeal to the Laboratory, and gradually decayed. Though I continued to work at the Laboratory for another half dozen years, until a lucrative early-retirement package came along, the research excitement at Livermore had definitely disappeared. The working population at the laboratory is now (at the end of 2008) only half its former size. My research from about 1994 through to the present has been carried out with my wife Carol and a large international group of collaborators from outside the laboratory.

VI. LESSONS LEARNED FROM LOOKING BACKWARD

My career at Livermore, with its many pleasant overseas interludes, left me with some powerful lessons, worth outlining here. They have to do with the value of research and its fruits and how it is best nurtured. *Publication* of *reproducible results* is the *sine qua non* of science. A research project, no matter how brilliant, is quite useless unless others can share its results. Coworkers, administrators, and editors are the filters through which work must pass before it enters the literature. Their suggestions are often good ones.

Some publications are not so good. George Stell suggested the journal name "Setbacks in Physics". Setbacks in Physics was to be devoted exclusively to faulty and incorrect solutions of significant problems already solved correctly in the literature. In my own research career I came across two sets of excellent candidate articles for that journal. Both candidates were in research areas where I had published extensively. A series of papers by Tuckerman and coworkers[36], pointedly ignored the simple relationship between Nosé-Hoover mechanics and the Second Law of Thermodynamics due to multifractal phase-space structures which I had described repeatedly in the literature. A second, remarkably long, paper by Zhou[37] was a specially effective setback, in that it spawned many successor setback papers, all pushing the original claim that the (wholly-correct) microscopic form of the Virial Theorem for the pressure was incorrect, and that the kinetic part of the pressure tensor should not be included.

A second category of "bad" paper, one with forged data, is more rare. The only example I came across myself was one Watanabe's free-energy calculation. His results were literally "too good to be true"[38]. A phonecall to his thesis advisor revealed that the computer program he used to generate free energies had wild fluctuations. The program was simply stopped when the free energy reached the "correct" value.

In the past good papers were often squelched by the review process. I remember Ed Jaynes had George Uhlenbeck's rejection of Ed's seminal paper on maximum-entropy theory framed in his Washington University office. Such defects of the reviewing process are not so important now. I have never failed to publish a rejected paper elsewhere. Because there are now so many outlets for publication, including the LANL arXiv and one's own website, arbitrary rejection is no longer a serious problem. Today an author can certainly publish if he wishes to do so.

A half-century of simulation work has left me with some lasting lessons. Reproducibility

is paramount, and Clarity is required. Scepticism and Openness are desirable, as is also a sense of Perspective. Visits and discussions with others most often lead to useful ideas. Publication is in the end absolutely necessary despite the occasional frustrations of peer review and the cronyism that discourages novelty.

For me the Livermore laboratory of the 1960s provided a nearly-ideal environment for learning about simulation – stimulating people, freedom to choose one's own way, plenty of secretarial support and computing equipment, the possibility of travel and publication. After a few years of microscopic simulations, first equilibrium and then nonequilibrium, as described here, it was natural for me to explore *continuum* methods to get beyond the limitations on system size and timescale posed by atomistic vibration lengths and times. The smooth-particle method, developed by Lucy and Monaghan in 1977 provides a method much like molecular dynamics for solving the continuum equations. But the particles are not necessarily small. They can be astrophysical in size. Smooth particles held my interest for many years, resulting in my most recent book, which is devoted to that technique.

A Japanese colleague, Shida-san Koichiro, a Lecturer at Musashi Institute of Technology in Tokyo, had been trained at Keio by Taisuke Boku and Toshio Kawai. We all met when Carol and I visited Keio in 1989-1990. Koichiro was able to work with us at Livermore on Maxwell's thermal-creep problem. He has very kindly translated all four of my books into Japanese. I am very grateful to him for this and suggest that the reader interested in more details of my work look for those books, either in English or in Japanese: [1] Molecular Dynamics; [2] Computational Statistical Mechanics; [3] Time Reversibility, Computer Simulation, and Chaos; [4] Smooth Particle Applied Mechanics, the State of the Art. My website http://williamhoover.info also contains a wealth of technical information, including electronic forms of books [1], [2], and [4].

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