Berni J. Alder, Interview

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Foreword

Berni J. Alder was awarded the 2001 Bolzmann medal for inventing the technique of molecular dynamics simulation and showing that with such ”computer experiments” important discoveries in the field of statistical mechanics can be made, in particular the melting/crystallization transition of hard spheres and the long-time decay of auto-correlation functions in fluids. He has also played a key role in the development of Monte Carlo methods, both classical and quantum.

Part I of this interview took place in Konstanz in the company of Giovanni Ciccotti and David Ceperley, on 9 September 2001, the eve of the *SIMU* conference “Bridging the Time-Scale Gap”. Part II was originally scheduled for the evening of September 11, 2001, and for obvious reasons, was postponed. It was completed in Berkeley during the mini-statistical mechanics meeting organized by David Chandler, January 2002. Conducting this interview has been a pleasurable duty for us, which we hope you will enjoy.

Dónal Mac Kernan and Michel Mareschal

CECAM,

Lyon, March 2002

To distinguish the interlocutors, we have used the following key.

Plain text : Berni Alder; **bold text G:** Giovanni Ciccotti; **D.C:** David Ceperley;

D: Dónal Mac Kernan; **M:** Michel Mareshal.

Part I

The Early Years

D: Berni, can you tell us about your childhood in Germany before you went to Switzerland ?

Yes, I lived in Duisburg for about eight years, and left in 1933.

D: Do you remember the atmosphere then ?

It was pre-Hitler. A fortunate fact was that my father was a manager of an Aluminum of America company. They tried to make aluminum in that area because there was enough power, and the Norwegians could bring in the bauxite by ship. The company collapsed just before Hitler came to power, and my father decided that we should move to Switzerland.

D: You were originally a Swiss citizen, so your father went there because it was useful for this aluminum plant ?

He got a very good job in Duisberg. We were upper-middle class, each child had a maid, so we had three. I have two brothers, one is my twin brother by the way.

D: What's your twin brother doing ?

He's a dentist in Berkeley.

M: A real twin ?

No, we are not identical twins.

D: So you always stayed in the same place ?

Yes, we have always lived close together. My older brother is in Davis. He's a mathematician.

G: Just what you are not ?

Yes, a mathematician in the strict sense. He's a number theorist. In those days it was easier to get jobs. If you lived in an area, you got jobs there. Nowadays, you have to move across the country to get a job. So, we all found jobs in the Bay area eventually.

D: You don't have any memories of Nazism in Germany before the war ?

Anti-semitism was there, but I was too young to really notice it.

G: But you remember the name of your nanny ?

Yes, Anna.

G: And she was German ?

Of course. You didn’t have to import your maids from Turkey then, as it is now.

D: Did you consider yourself Swiss or German ?

Swiss.

D: And then you went to Switzerland. Why ?

Well, my father saw Hitler coming.

D: So while you were not aware of it, your father was ?

Of course. I mean he saw Hitler coming, and anyway he had to change jobs, so he decided that he might as well leave.

D: How long did you spend in Switzerland ?

Eight years, from when I was eight until sixteen. We left in 1941.

G: So your mother and father left for California?

Yes, the whole family left. It was very hard to get visas at the time. The United States did not accept immigrants on the basis of nationality, but on the place of birth. As my parents were both born in Germany, they had to go in the German quota, which was jammed with people wanting to get into the United States. It took about two years of negotiations.

G: But America was already at war with Germany ?

No, it was just before. Actually, you had to go by sealed train through France to Spain, and then take an American boat from Lisbon. A German U boat stopped the ship on the high seas, and boarded it. It was dangerous. They shot a warning shot over the bow, and stopped us. They let everybody go.

D: And the sealed trains, from Switzerland to Spain, they were really sealed ? You couldn’t get out ?

Well, we stopped at one station and they let us get something to eat. All I remember was they had some chicory coffee which was undrinkable.

D: Do you have any memories of school in Switzerland ?

Yes, those were the formative years. I started school at grammar school (our second grade), and went half way through Gymnasium. I think that formed more of my character than anything else. You really learn there disciplined learning. In the first three years you take Latin, it was really very rigorous. It tends to make you focus on the essentials. I like the simple, down to earth Swiss approach. By the way, I was in Zurich.

D: Were there any subjects that you found particularly fascinating ?

You mean how did I get started in science ?

D: No, not necessarily, it could be science, history, art, almost anything.

No, it was a very general education, I wasn't pulled towards anything specific.

G: Were you lazy ?

Absolutely. That's an essential characteristic. Do the minimum amount of work to get by.

G: Were you good at taking notes ?

I cribbed, you have to be clever to pass exams with the minimum of effort.

M: You had Greek too ?

Well, I just left before, but wouldn't have taken it anyway, as the Greek option of the Gymnasium was the humanities, and the other one, more physics and engineering did not include Greek. It was an all boys school. The distraction of girls was not present. I think it has completely changed now.

D: And why did you leave Switzerland ?

It was too dangerous for my father. Switzerland was surrounded by Germany, occupied France and Italy, and in 1940 it was hard to foresee how long that war was going to last.

G: So the Swiss were anxious about being able to stay in power ?

I remember one time the German army massed on the German-Swiss border, and about half the population went to Geneva. I don't know if it would have done any good. People were really afraid. The Swiss claim that they were kept un-occupied because the Germans wanted the Gotthard pass intact. The Swiss had the plan to retreat to the mountains the moment the Germans came in. There was total mobilization. I was just sixteen, my brother who was 18 was already send to the frontier. The sixteen olds were drafted to help out on the farms, because all the soldiers were guarding the frontiers. It was back-breaking work. I remember pulling sugar-beet out of the ground, and the end of the day you were exhausted.

D: How many people were on this boat, and how long did it take ?

It took 5 or 6 days to get from Lisbon to New York. It left in April 1941.

D: And then you went to Berkeley directly. Why directly ?

I had an uncle who was an M.D. in Germany. In 1937 he took a trip to the United States, as he knew he was going to emigrate. He traveled all over the Unites States to find the most favourable place to settle. So he decided on Berkeley and went back to Germany and in 1938 emigrated to Berkeley.

D: How Jewish was your family, was it orthodox or reform ?

It was a typical German assimilating family. Thats of course the tragedy of it all. In the 20's German Jews tried to assimilate, to be more German than the Germans themselves. It didn't do them any good.

D: I heard that Jews in Germany during the first world war had the highest number of medals per capita ?

Yes, my uncle, the one that went to Berkeley had an iron cross in world war I. He was an M.D. and I guess he helped save some wounded during the war in Belgium. My father was totally areligious. He didn't eat Kosher food, and never set foot in a synagogue.

D: When you went to Berkeley, you were still basically a German speaker ?

Yes, I didn't speak a word of English. I had taken French and Latin in school, but didn't know any English.

D: So how long did it take you to learn English ?

Three months. When you are young, you learn languages very fast.

D: You were then in high school ?

Yes, I was in the last year of high-school.

D: And how did you find your first year in the States. Was it difficult or easy ?

Well you are young and adaptable. My parents had a much more difficult time adjusting then I did. High-school was extremely easy having just come through gymnasium, so my first year was just learning English. We were these odd Swiss twins, and treated very well.

D: And you still didn't get interested in physics or chemistry ?

Well, that was the typical parent's thing pushing to have a career. The same push that Teller and Wigner and Von Karman had from their parents to study chemical engineering because it was practical. Parents have a very strong influence in choosing your career. My brother studied chemistry also but eventually rebelled, and went into math.

D: So it was your father that was pushing to do chemistry ?

Yes, actually my father also had a Phd in chemistry from Munich, and he could not get an academic position because he was Jewish. Munich was very strongly anti-semitic.

G: And your mother, she also did well in her studies ?

No. She was born in a very small village, Hemer in Germany, and came from a typical profession that was accessible to Jewish people, horse handlers and butchers. She never had a chance of an education.

G: So your father was a manager in chemical engineering ?

He couldn't get an academic position due to anti-semitism, although he wanted one, so he took his first job in a brewery in Czechoslovakia, and that lasted for a year or two.

G: Was he very sad for not having pursued an academic career ?

Yes, he regretted that very much.

D: Did you start to study chemistry immediately when you started in Berkeley ?

Yes. I started university in 1942. There was a very compressed curriculum. I started in 42, majored in chemistry. The studies were very intensive due to the war, and by 44 I was already a junior, I was doing very well in chemistry, except for breaking test tubes.

D: That was everything, organic chemistry included ?

Yes, I had taken the organic chemistry course, and decided that I wasn't going to be a chemist. But the people thought that I was sufficiently good that they tried to get me out of the draft. I was a Swiss citizen in the United States, but everyone got drafted even if you were a foreigner, because the argument was that if you have the intention of becoming a U.S. citizen, then you had to go to the military, or go back where you came from, which in our case was Switzerland, and there was no choice. They tried to get me out of the draft because in chemistry in Berkeley, Seaborg and company had a branch of the Manhattan project. But I was just slightly too young, they wrote very strong letters trying to keep me out of the draft, but it didn't work.

D: Who was writing the letters ?

Latimer and Pitzer. These were chemists that were very prominent in the Manhattan project. Latimer was very powerful, and eventually testified against Oppenheimer. He was a very close buddy of Lawerence.

D: So you eventually had to go to the navy ?

That's right. You couldn't become an officer because you were a foreigner, so the only choice that you had was to go to electronics school. You had to go to boot camp, and that nonsense, but as soon was that was over they sent you for a year's schooling for radar. There were two important things then, the Manhattan project and radar.

D: Did you like your time in the navy, or did you consider it just a waste of time ?

I tried to get out of it as soon as possible. It was an adventure for a young man, but it clearly wasn't my cup of tea.

G: Were you good with radar ?

Oh yes. During the year of schooling you went to Chicago, and Treasure Island and Monterey, and then we were shipped out to Manila in the Philipines.

G: Was it an elementary thing or was it more ?

It was just after MacArthur had reconquered the Philipines. They established a communications centre for the entire pacific, all aircraft, all ships, all submarines; the station was just outside Manila. It was there before the Japanese invaded, so we established a whole radar station.

D: So you were there ?

Yeah, I was in the jungles of the Philipines.

D: What kinds of things were you actually doing there ?

Well, I could fix, and install all sorts of radar equipment.

G: And were you good at it, and does it have some bearing with your work on computers ?

That helped. There was one main thing I remember that was amusing. The station was outside Manila, and because it was a huge radar installation, they put it outside the city, but the headquarters was in Manila itself. So you had a cable that went between the two. They used an old Japanese cable, which when it rained, shorted out, and the entire pacific fleet and all aircraft could not be communicated with.

D: It rains pretty often in the Philipines ?

Yeah.

G: When you arrived in the Philipines Manila was already conquered ?

Manila wasn't liberated I believe when we first arrived, so we landed somewhere in the jungles. There were still Japanese gorillas there. It wasn't very dangerous, but you still had to be careful. Then Manila was taken, and we moved into the Manila area.

D: I would like to go Berkeley. What was the environment like scientifically as an undergraduate ?

It was extremely intense. The war was on, you just worked, there was no social life. Actually, as a junior, they were so short of manpower that I had to teach the freshmen, even though I had taken the course just a year before.

G: But somewhere you write that you were in the navy until 1946?

Yes, I came back to Berkeley after the war as an undergraduate, and finished. They tried to get all the veterans back to university. I was on the G.I. bill. Everybody tried to make up for the time lost. So I stayed on as a chemist for another year. I knew I didn't like chemistry, and did a masters in chemical engineering, while trying to decide what to do, and finished very fast around 48. Somebody recommended CalTech to do chemical physics. You see, Berkeley had a very anti-theory atmosphere, so I couldn't stay on there, and had to go.

G: So the professors in Berkeley didn't impress you too much ?

There were no real theorists there.

G: You don't have any scientific fathers from that period ?

Well, there were people who really liked me, and got me back to Berkeley after CalTech. A man called Jura. I once took his course, and I wrote a little paper, and he loved it. He liked me, but he wasn't really a theorist. I have a very poor opinion of theory at that time in Berkeley. Hildebrand was really the one who helped me.

G: But he helped you in the career, or he was inspiring in his teaching ?

I really liked Hildebrand. He helped me in my career, and of course he got me interested in liquids. He made me think about the problems of liquids, but he really didn't help me theoretically, as he was really into thermodynamics. I liked his personality. He was a great egotist, but he was a very great person nevertheless.

G: Göethe called this selective affinities. So CalTech had a completely different atmosphere from Berkeley ?

Oh yes, Tolman, Kirkwood, and Pauling were there. They were people who had an enormous influence.

G: There you were really challenged ?

Oh yeah.

From Kirkwood Integral Theory to Monte Carlo and Molecular Dynamics

D: How did you come to work with Kirkwood ?

I really wanted to work with Pauling, but Pauling wasn't taking any students. Well, he was willing to take me, but Pauling and Kirkwood argued, and decided that I should work with Kirkwood.

G: Which in a sense was better ?

I think so, Kirkwood was really very rigorous. Pauling was really much more intuitive. So Kirkwood was the supervisor of my thesis. I was one of the pupils of the school of Kirkwood. It was extremely challenging.

G: How old was Kirkwood then ?

He must have been about 45. He died very young, about 55, of cancer.

G: So he was still very strong ?

Yes. He was only in CalTech for 4 or 5 years, and I managed to do my thesis with him in three years.

D: And what things were you doing ?

The first thing that happened when I got there was that Tolman had just died. Tolman was one of the great statistical mechanicians. It was Kirkwood's job to write up the papers that Tollman had nearly finished. He actually worked on surface chemistry.

G: And Kirkwood was very energetic ?

Oh yeah. He and Joe Mayer, Debye and Onsager were probably the leading crew.

D: I told you before, that in Joe Mayer's archives there are some letters between him and you. So how did you get to meet him ?

I can't tell you how I got to meet him, but I got to know him really well, and also his wife Maria Goeppert Mayer. I used to visit them a lot in their house in San Diego. I guess it just came out of professional connections. We used to worry about virial coefficients. Mayer was someone you could just sit down and talk to. He was someone who could just enter your problem.

D: How old was he then ?

He was about 50, about the same age as Kirkwood. Anyway, we became personal friends, and also with Maria. There was also a connection between Teller and Maria. I used to talk a lot with Maria. I'll tell you an interesting story, given what we've been saying about Germany. You know she was German. Joe met her in Germany as a student. She was very shy, she would always sit in a corner during a big party, no one would talk with her, as it was hard to make small talk conversations with her. So I used to sit down and talk with her, and I guess thats how we met. The thing that I remember her telling me was this. As you know she won the Nobel prize, and she said that she would have given away the Nobel prize if she had had the ability to make small talk. Its amazing, because her mother came from an upper middle class German family. At that time all you had was tea parties, that was your social life. She envied her mothers ability to make small talk, which she never could do. Eventually they drank more than they should have, and it got rather unpleasant.

G: You were going to talk about your thesis, and then you jumped

The major part of the thesis was Kirkwood's theory of thermal conductivity. The only part that I can remember writing up was an extremely elaborate formal theory.

G: It was the most difficult part of the work of Kirkwood, trying to get dynamical properties from equilibrium.

Yeah, from the friction constants. It was totally wrong. I found it rather painful. It was totally uncontrolled.

G: Not many papers came out of your thesis then ?

Yes, but one thing that came out which was pretty influential was some work I did with Irwin.

G: Irwin and Kirkwood 1950 ?

Yes, I worked with Irwin on that paper. Irwin was the sort of guy that never wrote up his Phd thesis, a brilliant guy, and that was really a brilliant piece of work.

G: I thought it was Kirkwood ?

No, it was partly at least Irwin. Irwin hated to write up things, as I said he never wrote up his thesis. Irwin impressed me enormously. The paper was simple, clear and clean.

G: It was giving really the correspondence between microscopic and macroscopic in a very beautiful way

M: Irwin was a student of Kirkwood ?

He was intellectually a post-doc, I think he went to Princeton but he never wrote up his thesis. I think he drifted into industry afterwards. Irwin contributed at least half to that paper. Kirkwood did not always write in a clean and clear way.

M: So the thesis was completely theoretical, there was nothing numerical in it ?

Well, half the thesis was this Kirkwood theory, and the other half was calculating the radial distribution function for hard spheres from the Born-Green-Kirkwood-Yvon equation. Thats how I got started in numerical stuff actually. I also worked with a post-doc called Maun. He was a post-doc that had already started trying to solve these non-linear integral equations for the radial distribution function. That's why you got punching the Marchant machine, or what ever it was in those days.

D: And how did you actually do the numerical equations then ?

You grind. You do mechanically what you now you do electronically. We used, a Friedan Marchant machine. Its an electo-mechanical device. Actually for some reason, I still have Kirkwood's own computing machine in my house. I kept it for historical reasons. For some reason, when he died or left CalTech I inherited it. Nobody wanted it. Its not that big.

Anyway, that was a really crucial experience, because that's how I eventually went to the CalTech computing centre. You see, Maun did most of the work, and unfortunately went insane, so I decided to go to the computer centre, where I met Stan Frankel. He also disappeared from the scene like Irwin, so many bright people disappear. He came to CalTech from Los Alamos in around 1948. He was in charge of the computing centre, which were these IBM machines using cards. He was very clever. He was the first one to talk to me about Monte Carlo, because in Los Alamos, he had worked on electronics.

G: So if he was there, that was the short circuit. Kirkwood was very much opposed to numerics ?

Yes, Kirkwood was in love with his integral equations, but needed to numerically solve them. This is a long story. The first thing we did with Monte Carlo was just put in trial particles at random, and if it didn't get in, we rejected it, and tried again.

G: It was uniform Monte Carlo ?

Yes, and so you never get to high densities. We recognised that after one trial, and started putting them in a solid lattice, and juggled it. Hard spheres are extremely simple, and the only question is, of course, detailed balance. When it doesn't get accepted and you put it back, you have to count that configuration again. For some reason, Kirkwood would never accept this as being detailed balance, and that's one of the reasons why we never published it. Another reason is that Stan Frankel and I left CalTech. Frankel and I did eventually publish a paper on it, maybe three or four years after Metropolis, Rosenbluth, Rosenbluth, Teller and Teller. This was around 1953-54, in the Journal of Chemical Physics. Kirkwood would never accept it until Bill Wood through his probabilistic arguments convinced him that it worked. We clearly did not have enough power to do a lot of Monte Carlo moves, and we chose a solid phase to actually get the radial distribution function. Frankel went to Manchester, to the Feranti machine, because that was the first accessible electronic machine. He went there for a summer, and still didn't get enough statistics. Then Livermore was established around 52/53, and of course Teller knew we had done this work. If you look at the original Metropolis paper, he acknowledges that we had developed an equivalent method in a footnote.

G: Sorry, when did you leave CalTech?

In 1951, I then became a full time instructor in Berkeley in chemistry. After three years as an instructor, I took a Guggenheim fellowship to Europe, around 54/55, and spent half a year in Leiden, and half a year in Cambridge. Leiden, because statistical mechanics was very strong in Holland in those days. Mazur, de Groot, and one of the old timers. It was very strong atmosphere, Uhlenbeck and Pauli came. I remember it as a very active centre. In Cambridge I went to work with Lennard Jones. He left to become some “big cheese” in another university. But I did work with Pople quite a bit, and Longuet Higgins. It was a very good time.

D: What sorts of things were you doing then ?

Oh, I was piddling with Virial coefficients, mixtures and dielectrics. The usual thing you do after your thesis, a little more of it.

G: But your thesis wasn’t exactly on that. You had found these simple properties related to the radial distribution function, more interesting than Kirkwoods theory of conductivity etc.

I didn’t pursue the radial distribution function except for mixtures.

G: This virial, you got from somebody, or it was your way apply what you had learned.

Actually, what happened there is that I spent more time doing experiments with Hildebrand’s group, than anything else. They wanted me to help interpret their results.

G: It was much more Mayer’s style what you were doing than Kirkwood’s.

Right. I didn’t pursue transport, I found it too complex, and wrong.

G: Who helped you in changing this perspective ?

Well, I think Hildebrand had an enormous influence. Let me tell you something that few people know. He suspended some jelly in a fluid of the same density, shook it up, took pictures and got a radial distribution function out of it. That was done in the thirties.

G: That was very smart.

Somewhere along the line David Turnbull at Harvard was shaking balls on a two dimensional surface, and taking pictures, and when he heard about our numerical discs, he gave up. He became a tremendous supporter of Monte Carlo after that. Do you know him ?

D: Ahh yes, he sent Charles Bennett to you right ?

I can’t remember if he sent Charles Bennett to me, or if Bennett decided by himself to come.

G: And aside from supporting it, did Turnbull end up doing simulation himself ?

No, except through Bennett.

G: So in Europe, you were a kind of Uhlenbeck expansion man for mixtures, virial, this kind of thing?

Yes. The other thing I got involved in at that time was dielectrics, with Pople and Buckingham.

G: You published something with Buckingham ?

No, it was one of the most confusing messes that I have ever been in. Kirkwood had worked on di-electrics, Onsager had, but they didn't have the right model, or the right theory. When you have a permanent dipole it was okay, but when you have polarizable and permanent dipoles, it turns into a huge theoretical mess. Pople was working on it, and I think Buckingham was a student.

D: How did you get involved in M.D. ?

That was in Livermore. I came back from my Guggenheim, and Livermore then started to have machines, and Berkeley chemistry was not particularly suitable to me. But I have still to this day a connection to Berkeley chemistry. They gave me an office, and treated me very well. I drifted off to Livermore, partly at first as a consultant. In fact I was a consultant there before I left for Europe. I think Teller persuaded me, because he knew of our hard sphere work which was applicable to equations of state. He knew about the hard sphere's integral equations, and also about the Monte Carlo hard spheres. Anyway, it turned out that anybody who could walk went to Livermore in those days. He tried to persuade me to be a consultant, and it turned out that I was the consultant for equations of state at Livermore. Before I went on the Guggenheim, and when I came back I worked on very high density problems.

G: But apart from this episode of Monte Carlo, in Europe you were strictly analytical ?

No, I gave lectures on Monte Carlo. I do remember talking in Cambridge, and at the Lorenz colloquium in Leiden. But there was no machine, so what could you do ? You can talk about it, but with Monte Carlo thats a game.

G: While playing with this Monte Carlo at the beginning, you had already set up the system with periodic boundary conditions ?

Ahh yes, periodic boundary conditions came immediately.

G: So the general situation of a simulation was already thought of at the moment of the Monte Carlo ?

Yes, by 1950, we already had used periodic boundary conditions.

G: Kirkwood didn't trust this sort of thing, how about Frankel. Who had this in mind ? This is very strange, that people wanted to do a small box to do statistical mechanics for $g(r)$. Its very strange, so you have it to explain to us.

D.C. : Wasn't there a lot of skepticism that with a few particles one could simulate a liquid ?

G: Frankel came to Europe, and he was able to do Monte Carlo, in the sense that he had to solve an integral, which he could do by Monte Carlo. But, then you started a much more dangerous game, where you filled the box with particles. This was a big jump.

Well, the big problem was: is there a phase transition ? You see the integral equations were miserable, their stability was so horrendous that you become desperate. So what do you do ? You think of the Monte Carlo game

G: But in those years it was not evident to do particles, it was laughable, and to do phase transitions, to try to see the phase transition was not natural, and Kirkwood was not stupid.

D.C. What was Kirkwood's main objection ?

Kirkwoods main objection was that he did not believe that we obeyed detailed balance in our algorithm

G: In other words, Kirkwood was in favour of trying under the condition that you could satisfy detailed balance. To my knowledge he was opposed.

He was opposed. You know I don't know his psychology, but he really believed in his integral equations.

G: That that would bring him to the phase transition ? He was really to bright to believe that, due to one of the most stupid of things. You know that things de-correlate, and yet you know that at the phase transition they correlate very much. He already knew that, this is what you assume

No, Kirkwood's mind was rather mathematical, he was more a formalist. He saw the density splitting when you get to the singularity was probably reliable in his integral equation method. His transport theories are very formal, and I think psychologically he did not like an upstart new-coming method to beat you.

G: So you were young and foolish, Frankel was a little older than you, but was not a realized statistical mechanician. To have solved this problem, you would have been happy to arrive at some approximation. Instead, you started toughly to say, I put 22 particles, the density is the good one, and those stupid particles crystalize or rarify. It's some jump. Now it's so trivial.

But they didn't solidify. The system was too small. How did we dare do one hundred particles in a box.

G: Yes, this is the really question you have to answer, because you have already taken the box sum so you don't have to convince others that you are bright. So now you can be sincere, and tell us what the hell you had in mind.

Well, I can't really give you the train of thought.

D: You just decided to give it a try ?

Yeah, you give it a try. We were extremely unhappy about the lack of stability of the nonlinear integral equations. And so I think talking with Frankel, we just decided to try something else.

G: You have a bad memory, but I am sure that you started being with this poor Frankel that knew he could fit particles in a box. So a box, ahh thats interesting, how was your appetite growing and you were even dreaming to represent the transition, its so strange.

Well, we tried one particle at a time.

G: And of course you realized that if you were putting them in a crystal, they were staying in a crystal. Now you are saying that in a crystal, they are just immobile. Okay, now let me start them moving, and if they move much will they liquify, and then you thought, ahh this is statistical mechanics. That's a jump, because this was a game, now there are regular, then they go irregular. When did you think , oh shit this is a phase transition ?

I can't remember. You just slide into this. I think we must have first tried the particles in a box, and we had a certain periodic box already there, and we already thought that we had a limited number of particles, and we thought that if that doesn't work, just put them in an irregular **??** way. That's my recollection of it.

G: But, you must remember a moment of extreme joy when you said "porca" we have got something really important ?

Yeah, but let me tell you something. When we did this in 1949/1950, and in 1951, I left CalTech without any results. Then the Metropolis thing came, and they missed the transition. At that time my argument was they had done Monte Carlo, and they had missed it, so lets try something else, and that how I started molecular dynamics. I wasn't going to repeat their results.

G: Be calm, lets stick to Monte Carlo. You didn't have convincing results of anything, and moreover you weren't sure of having the right detailed balance mechanism, because Kirkwood was critical and in part because there were no good machines, and you continued to think of this mentally, and then you went to Europe where you did analytical games. Then, when the paper by Metropolis came out

Teller had probably told me about it.

G: But without having the proper information about the melting/fusion transition, you knew they had got the right Monte Carlo, and you understood that the mechanism could exist.

These were great authorities, who had duplicated our method, and had not found the transition.

G: You were confirmed that the possibility to play the game was there, although perhaps it was low, it was not good enough. The phenomenon was not there. Now you tell us that you decided to try something different.

M: Just wait a moment. The algorithm that you were using was already a specimen of this, and with overlapping you would reject this move, but you would accept any move that would lead to non-overlapping ?

Of course

M: So it was basically the same algorithm.

Yes, we would accept any move that would not lead to an overlap. And if it did lead to an overlap, we would reject the move. It was clear that we had to count the rejected configuration for detailed balance. We didn't call it detailed balance. The ideas were very clear. If you have a configuration, and you try, and you try and you try, and every move gets rejected, than it must be more probable. It just intuitive.

G: The real question was only should I keep the configuration rejected in the sample, or not. It appeared in this way. The question of the detailed balance was what I do with the most intuitive thing, and it disappears from my sample. The statistical mechanical one tells I reject, which means I stay where I am, and I have two configurations which are where I am. So the confusing question was, what is the proper sampling. They didn't see clearly what to do with this rejected configuration. Perhaps they corrected it, now I don't know. The formulation of this was clear, although it was not stated.

No, we didn't use it in terms of detailed balance. The argument was very simple, I think I just said it. If you have a configuration, and every move you make gets rejected, that means that the probability of the configuration which you came from is a very probable one. Thats the natural thing to do. We didn't put it in terms of detailed balance, or a formal theory.

M: Somehow molecular dynamics was for you another way of having a good sampling

No, molecular dynamics for me was just another way to get at the hard sphere phase transition, at the beginning.

G: How and in which circumstances, you did the reconstruction. Even though Kirkwood was a very serious teacher, I am sure that ergodic theory and all those things,

arrived to you in a very confused way.

Why ?

G: Although a good book of statistical mechanics starts with dynamics and the Liouville equation, Giorgio Careri in 1979 didn't understand how molecular dynamics could do equilibrium statistics, because this is dynamics, so what has it to do with equilibrium. He's a confused mind in general, but anyway this means something anyway. In 51 or 52 or 53, when you started to think of this thing, the idea that you could realize the phase space trajectory of hard spheres, and from that from time average get the phenomenon, or if you want by simply looking get the melting. It is true that perhaps you didn't want to see the average properties at that time, but just the phenomenon of the dis-ordering, the melting. Is this the key ?

The motivation at the very beginning was to see the equilibrium.

G: And the dynamics could be the key of the going ?

Yes.

G: Ahh, so you were Correllians, the dynamics would change my configuration ?

No, we were thinking of the phase transition. I don't think we even thought of molecular dynamics this way. Are you implying that it might cover ergodic phase space more efficiently than Monte Carlo ?

G: Ahhh, you didn't think of that perhaps ?

Well, we worried about it. Actually the very first thing we probably did with molecular dynamics was not go after the phase transition, but we went after H- theorems and compared it to Monte Carlo in terms of efficiency.

G: That's strange, because no one from what you told up to now, taught you on such a thing, because Kirkwood was teaching statistical mechanics, that's true, but also much thermodynamics. For example, he was busy with transport, but not so much with relaxation to equilibrium. He was not an ergodic theory man.

No, he did certainly made me aware that ergodic theorems are never proven, in the sense of time averages. I took his courses. He was very careful.

G: Ahh, so he told you about the Boltzmann equation, the H theorem, etc ?

Oh yeah.

G: In his books you don't find any of that.

Yes, but his course had all of that.

M: And irreversability ?

Yeah, irreversability, and the theory of measurement, and Brownian motion, all the fundamentals. I was aware of all that. It's interesting that the first application of molecular dynamics was for H-theorem's. Kittel, for example who was in the physics department at Berkeley got extremely enthusiastic, and put it in his book.

M: You came to Brussels to talk about that.

Yeah, Prigogine. That's very interesting. We were flown by an air force plane, Von Karman ran that conference anyway. There was an airplane for all the people that came to Brussels. Kirkwood, Mayer, and others were on that plane. And when Kirkwood heard of this molecular dynamics method, he was extremely enthusiastic. He jumped on it. He didn't threaten me with his integral equations. He thought that molecular dynamics was a deep contribution. So he accepted it. I remember talking to him for hours on the plane from Washington to Brussels about the paper I was about to present.

G: Ahhh, and then he died, because he could have been extremely instrumental in getting molecular simulation widely accepted. I think that was 56. I came back to Livermore in 55, so we had just developed molecular dynamics, and so it took us a while to get it going. So it must have been our very first results, which we presented at the 56 Brussels conference.

G: Okay. So you tell us that molecular dynamics was first applied to the relaxation to equilibrium. So how did it come to your mind to solve the equations of motion of the classical mechanics as something to do science ?

Well, there were two motivations. First see if the Los Alamos people had done the Monte Carlo dynamics right for the phase transition.

G: That was later on.

That was later on. I'll tell you why. It took a massive amount of machine time at that point.

G: But I want to say that you already had the mechanism of molecular dynamics in your hand when you tried to match the calculations of the Los Alamos people, and it was not so simple.

Yes.

D: Actually, that brings us to another interesting question. Were there other incidents of people doing molecular dynamics before, in isolated ways which were disorganized ?

Yes, there's the Fermi-Pasta-Ulam experiment.

G: Were you aware of the Fermi-Pasta-Ulam experiment, as it came out in 55 ?

Probably not.

G: What were you aware of ?

The only thing that I was aware of was what Vineyard in Brookhaven did...

G: No, this is after, I think in ’59.

M: Fermi-Pasta-Ulam wasn’t even a paper, it was an internal Los Alamos report, so this could have been from before.

G: Yes, so you should clarify this for us.

I personally was not aware of any molecular dynamics.

G: Then, it’s not so natural that you imagine a programme to do molecular dynamics for hard spheres.

I must say that people (for example when I talked to Teller) originally thought molecular dynamics would be hopelessly computer intensive.

G: How did it get in to your mind to go to them and say, I want to do molecular dynamics ?

Well, I think my motivation was, “well damn it all, I want to see if hard-spheres by some other method has a phase transition. So, molecular dynamics was a clear easy alternative. But it took us a while to realize that it wasn’t all that complicated.

G: I don’t want to upend your method, I want to illuminate it. So I want to understand, you were with Tom Wainright, and instead of playing the goat, you now move the particles. That was not so normal. I mean the many-body dynamics terrorized Poincare. You had a miserable computer, good for nothing. you had to do billions of operations to do whatever, and you said, instead of playing the goat, I will do molecular dynamics. This is not normal. So somebody should have told you, for four-body I can do dynamics.

But for hard spheres you knew that they move in a straight line.

G: This was very bright. Its not immediate for someone that has studied some dynamics. You are also a chemist, so you studied Newtonian dynamics, which is a miserable way. So something around gave you the information, so tell us.

Well I think we just decided to try and doing it after we realized that it wasn’t so complicated.

G: Was Frankel a mathematician ?

Frankel wasn’t involved with this.

D.C.: Sorry, maybe I missed it. Who else was involved ?

Tom Wainright, he was a physicist

G: What did he bring to it?

Just energy and intelligence.

G: You have not told us when you met Wainright

Well, Wainright had an office not far from me in Livermore. This was after I came back from Europe. I was in Europe in 54 and came back in 55. We discussed a lot of problems. There was already a lot of work being done in hydrodynamics in Livermore.

M: You mean there were already particle methods for solving hydro-dynamical equations ? This is very interesting.

Oh yes, that was already developed after the war. Pic (particle in cell) methods were developed in Los Alamos by Harlow I guess in the late forties. Wainright did not have any particular back-round in statistical mechanics. He was one of these general physicists who had worked on weapons problems.

D: What was his back-round ?

He was a solid state physicist, from the mid-west.

G: So you discussed with him your mania of getting these particles to move, and he offered to you Newton ?

No, I think I brought Newton to him. He was just a sort of soul you talk to, and a problem solver. I said to him, why don't we see if we can do Newton, and we started talking. We then started thinking that hard spheres is much easier than solving Lennard Jones or whatever.

D.C. Who did the programming ?

Mary Ann. In those days physicists did not programme. There was no programme language, so it was done in machine language with IBM punch-cards. She had a bachelors degree in mathematics, so you had to give her very specific instructions how to do that.

D: Can you describe to us how the programming was done physically, as for most of us nowadays it is unimaginably complicated. What was the machine like and what was the basic process.

The programming was done in machine language. We had vacuum tubes. The machines were about the size of an ice-box. They only had a one hundred word memory. There were mercury delay lines and vacuum tubes, and oscilloscopes. I think we must have first programmed on Univac 1. The other huge problem which people don't face now, was the unreliability of

Figure II.1: Standing: Berni J. Alder. Seated: Mary Ann Mansigh and Tom Wainwright. Alder's office. ”We are looking at oscillograph traces from the computer generated motion of particles.”

the machines. If one positional velocity gets out of wack, you're lost. Anyway, neither Tom Wainright or I ever programmed. It took us a few months to do the programme. The pictures of the melting transition from the oscilloscope became very influential in getting the results accepted, they got in many professional text-books. That is interesting by the way, because later we made a film of irreversability, I think in the early sixties. I got a letter the other day from the guy who made Mathematica, Steve Wolfram. He said that he got totally inspired as a student by the pictures of the particles moving.

G: That represented an enormous jump in the attitudes of people.

D: But the major drive was to try to prove the existence of a melting transition in hard spheres

Yes, you must realize that in statistical mechanics, that was the 64 dollar question, which Uhlenbeck put up in every statistical mechanics meeting in those years. Everybody was driven by that.

M: So you had the velocity correlation function

I can't remember when we had the results. It took massive amount of computer time, and we probably did not have reliable results at that time. Actually to calculate transport coefficients by these autocorrelation functions was another good way to go. We actually exploited that right away, as we knew you could do it at any density, and had already presented it at the Brussels meeting. There was no theory at high density.

G: But linear response theory was developed for that in 56 ?

Yeah, but this was ahead of that.

D: I am getting confused about dates.

The history is that we did these H-functions, ergodicity and velocity correlation function before we went to a massive calculation on the phase transition. Only after that was done, did we go back to massive calculations on the velocity correlation functions.

M: Maybe the problem about the H-theorem and irreversability was more appealing ?

It was intellectually interesting and cheap computer-wise.

G: He got the enthusiasm of Kirkwood immediately.

Immediately.

M: And Prigogine too was very enthusiastic

Yes, Prigogine was enthusiastic.

G: I don't want to be offensive, but if Kirkwood had survived 5 years, the success of molecular dynamics and possibly Monte Carlo for statistical mechanics would have been speeded up by 20 years. While Prigogine is much less important.

I think Kirkwood was much more influential. Actually Joe Mayer was also very interested in the Monte Carlo methods. All these people in Los Alamos got involved.

G: Yes, but Kirkwood was an intellectual giant. If he had said to the Americans molecular dynamics is the way to go, it would have been a totally different earth.

Part II

M: Ok Berni, you read the notes by Dónal and we were at the time that you were going to report to a conference in Brussels in 1956. You were reporting the first results on molecular dynamics. You were reporting on the enthusiasm of the community reacting to this. We were saying that Kirkwood was an intellectual giant. If he had said to the American community that this is the way to go, that would have been a totally different earth.

Thats a statement of Ciccotti, I think. Yes, it certainly would have helped promote the method, but the method promoted itself very well. I think that its slow acceptance was because people didn't have the computers to get into the game. Very few people had access to computers and that delayed things. Kirkwood's enthusiasm would certainly have helped, but I think it would have only speeded things up a little bit.

M: That's one thing, but at the same time, they got access very rapidly. May be ten years later, everyone could have access to a computer and do molecular dynamics, but that did not happen so rapidly.

It took a while for it to get accepted intellectually.

M: What were the issues at that time ? It was the late fifties. You and Bill Wood came with the results for the transition to a solid phase from a fluid for hard spheres. That was a big step in the promotion of molecular dynamics

Yes, it answered the important physics question in statistical mechanics at the time: was there a liquid to solid phase transition for hard spheres. Analytically it was impossible to do anything about it. The numerical methods were the only way to tackle the problem. Having resolved an intellectual problem made the methodology acceptable. Of course, there has always been a resistance to use computers instead of theoretical methods. This feeling was very strong among the old timer physicists, to do things analytically instead of numerically.

M: Who were the big names? When you came to Brussels or Varenna, what kind of people were you addressing ?

Onsager, Uhlenbeck, Mayer, Debye, Kirkwood.

M: So, what was their reaction ?

I think they were all very positive. I have no recollection of any intellectual problems. Even Uhlenbeck, who was probably the most dominant person in the field, paedagogically speaking, certainly accepted the hard-sphere phase transition. These people also knew the difficulty of doing it analytically. This problem is yet to be done analytically, so they accepted the method.

M: Did they understand that the method could develop and make obsolete perturbation and expansion theories, approaches which were much developed at the same time ?

Well, Mayer was still hoping that the virial series would show a divergence, and kept hoping that it would. So they may have viewed this as an alternative way to show the phase transition. But they kept on going. Kirkwood kept on going with his integral equation singularities. People kept on doing what they had been doing. They accepted this as a temporary numerical result showing that there was a phase transition.

M: You were doing these things for hard spheres, one had to wait ten years until the paper by Anees Rahman was published on Lennard-Jones.

Verlet was already doing things with Lennard-Jones in the early sixties, I think. Verlet got into the continuous potential game very early. We did hard spheres for two reasons. The primary reason was that it was an order of magnitude faster to do molecular dynamics for hard spheres than for Lennard-Jones. So that's a very good reason, as the machines that we were using were just at the edge. Also there was the expectation, probably coming from Kirkwood, that hard spheres had the essence of the solid and liquid phases. Of course theoreticians were hoping to treat a hard-sphere system more easily than a continuous potential system. We considered continuous potential systems, but for numerical reasons, and because it is a simplified system, we decided on hard spheres. By the way we have always stuck to hard spheres in subsequent calculations. It does have the essence of the physics in it in the liquid phase and even the solid phase. One doesn't have to go to Lennard-Jones.

M: Except for the fluid-fluid.

Yes, but for that we used the square well. That's still much cheaper than Lennard-Jones.

M: You mean you did the square well fairly rapidly after hard spheres ?

Oh yes, we did it in '56 for Prigogines conference, because we were interested in the H-function for square wells. You see with square wells as you have only two discontinuities to worry about numerically, they weren't much more difficult than hard spheres. We quickly showed the gas-liquid transition for square wells.

M: Can I quote you in the proceedings of this 56' conference, you said that to show these phase transitions for continuous potentials would have taken years and years ?

It would certainly have been much slower. I think we figured out it was an order of magnitude faster to do hard spheres, which took many months.

M: And that was a reason for the community to continue to go on with virial and perturbation expansions. The fact that you were addressing hard spheres, and not regular potentials.

Well, at that time there was still the hope that something about the phase transition could be found from the virial coefficients, independent of the potential. But that hope has not been realized. So this is still the only method which shows for finite systems a solid-liquid phase transition. You know, hard spheres also made the following important point. In textbooks, when you look at the intermolecular potential, they always draw the Lennard-Jones potential, but the zero of the X-axis is never shown, and it is way over. So the repulsive potential is about twice the width of the attractive potential. All text books give a misconceived idea of the importance of the repulsive potential, because it is much broader than the typical graph shown of the Lennard-Jones potential. So what the hard-sphere phase transition showed was the vast importance of the repulsive potential in determining the structure of the system.

M: Yes, this reminds me of the result of Resibois and Piasecki that computing transport coefficients for hard spheres would be enough. They considered van der Waals long-range attractive forces, and they showed that the correction was something like two or three percent, which was really negligible. But that was for transport coefficients.

For transport coefficients, if you take the van der Waals model rigorously, you have a weak and constant long range potential, and the transport coefficients of that model are the transport coefficients of hard spheres. We did similar things to Resibois and Piasecki. We have several papers out comparing actual transport coefficients with hard-sphere transport coefficients. The most important correction is not the correction for the attractive potential in dense fluids, but to make the hard sphere diameter slightly temperature dependent. That softness of the repulsive potential is the major correction needed to get realistic transport coefficients. Hard spheres also emphasized that the repulsive forces are totally dominant in determining liquid structure. Much later, there was a beautiful piece of work by Daan Frenkel where he showed that you can get all these smectic and nematic phases, there are about ten different phases, you can get all the phases from purely repulsive potentials. I am amazed that it worked, even though it was what I had hoped.

M: So you have gone very rapidly into the transport coefficients. Transport coefficients I think was the first thing you addressed after the equation of state.

Yes, we spent about ten years on the hard sphere equation of state, and other equilibrium properties. We calculated for square well potentials the higher order corrections to the mean-field theory, due to the finite range of the square well potential. You can rigorously calculate the correction terms in powers of 1/T, where T is the temperature, and we determined that the series is converging extremely quickly, and is dominated by the 1/T van der Waals term. That all took us ten years. In the meantime, to go back to transport coefficients, the computers had improved enough, so that even though in 1956 we were able to calculate the velocity correlation function for the diffusion coefficient, but we could get only maybe 10 averages on the computer at that time. It took some ten years before we could do a very good averaging job, to get enough statistics on the velocity -velocity correlation functions, and on the others, stress and so on as well.

M: Wait a minute. The formula for the diffusion coefficient is an old formula due to Einstein. But for the other transport coefficients, we don't have such a clear formulation. so you had to wait for the theoretical framework to give you the relations.

Well, with hard spheres, when you have an impact, you cannot use the differential version of the fluctuation- dissipation theorem for the stress, because there is a kinetic and a potential stress term, and the potential - potential autocorrelation term diverges for the usual formulation of transport coefficients. So you have to use an integral version, and I found a paper by Gene Helfand in the late fifties/early sixties, with a proper integral formulation of the stress-stress and the thermal flux correlation functions in the spirit of the Einstein diffusion formulation.

M: So it was for the mean square displacement, rather than for the auto-correlation function ?

Yes, the equivalent of the diffusion equation is the mean-square displacement, so this was the equivalent of that for the stress and the thermal conductivity. So we had used those expressions already, but I am not sure how we started. We certainly started redoing the velocity auto-correlation function some ten years after the fifty six conference for hard spheres. By that time, we had enough statistics to see what is now called the long-time tail. That was in the mid-sixties.

M: That was much before publishing the paper. The paper was published in 1969.

Yes, we started in 1965/1966. It took us two years to figure out and believe this long-time tail. That's really one of the most qualitatively stunning results, and we just didn't believe it. How could a particle remember for some one hundred collisions its initial velocity. We did every possible test to make sure that the results were right. So we studied it for a bunch of densities, to find out when it occurred. You don't see it at lower densities because it is too weak, and you don't see it at high densities because the back scattering effect dominates at long times, that is for a hundred collisions, which was the longest we could study. Only at intermediate densities did you see this tail.

M: So you didn't believe it.

No, and we didn't publish it until we had a total explanation. That took several years. During the first year we realized that if correlations persist over one hundred collisions, you cannot explain it through kinetic theory. If you try to do the calculation collision by collision, after three collisions you run into horrendously complex analytical problems. So we finally decided, Tom Wainright and I, that the only way we could explain it was hydrodynamically, because it has sufficiently long time scales. And of course that was the key. Then we looked for an analytical solution of a sphere moving in a fluid, which is a standard friction problem.

M: That was solved by Boussinesque ?

It was solved by Stokes, in the late eighteen hundred's. They already knew that a sphere in two dimensions would have this vortex back flow forever. However, we could not find an analytical solution for this tail within hydrodynamics. I quickly came to the conclusion through a dimensional analysis that it had to fall off as 1/t , t being the time and in two dimensions first of all. You can do an extremely simple dimensional analysis to get the 1/t, but to get the coefficient in front, A/t, what that A was, we could not find an analytical solution. So we did a hydrodynamical problem numerically to get the coefficient, and then Tom Wainright who is better at analysis than I am, worked out the A. So, we first showed that it was dropping off as 1/t, and then the value of the coefficient, and only then did we publish. We talked about it first at a statistical mechanics conference in Kyoto in sixty eight. I remember that Kubo got sick, and needed a replacement to give his talk which was for a half-hour. People knew we had interesting results, and they gave me his spot. People were still not quite believing it, because they believed in Einstein, that the particle would forget its past-history, as a Markov process.

M: People believed that all correlation functions should decay exponentially, and that there is no algebraic decay.

Absolutely, everybody believed that, including Einstein. That's why we took so long to publish, to make sure that we were not being misled by some numerics.

M: But during all this time, you were discussing the result with people and trying to get an interaction going ?

No, only with Tom Wainright.

M: So you did not discuss it with Eddy Cohen or Bob Dorfmann or Pierre Resibois or Matthieu Ernst, or all the kinetic theory people ?

Well, clearly kinetic theory was useless, it's hydrodynamics, right ? Kinetic theory can not do things for more than a few collisions analytically. So I felt that was useless. We had to get our own hydrodynamics solution. So just Tom Wainright and I talked about it.

M: But at the same time they were trying to develop transport coefficient as a density expansion, and they were facing the difficulties that were connected to what you were doing.

Yes, I knew that Eddy Cohen had found out that there was something fishy with the virial expansion for the transport coefficient, and that they had spent a long time working out logarithmic terms to the corrections. I knew all about that. Clearly there was a difficulty, but they were doing their thing, and we were doing ours. It was a totally different approach. Then, of course, Eddy Cohen was at Kyoto, and he immediately accepted it, and within two days using a graph approach did what had taken us almost a year. He had not only the 1/t but also the coefficient. It turns out that we had made a small mistake, Tom Wainright had missed a pi somewhere in our calculation, and when he corrected it, the results agreed. So the stuff that Eddy Cohen had done was very close to what we had been doing. He had to sum these ring graphs that showed that the information was fed back to the particle, which physically is similar to our explanation. And then it turned out that Pomeau for plasmas had already in a paper two years earlier shown that there was a 1/t power law. I don't know if you know that.

M: Yes, I know about a model of discrete velocities he had. I think it was even in his thesis. The story that I know was that his thesis promoter was Yvon, the Y of BBKY.

He was a great physicist.

M: A great physicist, but also a French mandarin, very traditional and conservative, and he would dismiss results of Pomeau by saying that you've done a mistake.

It's not believable !

M: Then Pomeau came to Brussels to ask Resobois for advice, and Resibois said your computation is correct, you can present your thesis and I will talk to Yvon. So Resibois did not participate in the calculation, he just checked it.

I only found out about Pomeau after we had done that. But you see when you get a result like that, you just don't believe it, and we spend two years checking it.

M: So what did you first think, it was an effect of the model ?

Well there are all sorts of possible errors. You don't conserve momentum exactly or whatever. We just kept shut up as we didn't believe it ourselves, until we had a convincing computer demonstration and an analytic explanation for the tail, and then everyone accepted it. Well, almost everyone. I am sure Resibois and Pomeau, and Eddy Cohen and Dorfmann believed it.

M: But your paper was not accepted right away by Physical Review Letters?

Ahh, I forgot that, that's right, Physical Review Letters rejected it. Some reviewer did not believe it.

M: It was rejected , and then you decided to fight back with the referee.

Oh no, I think it was published in Physical Review. I don't fight Physical Review Letters. I can't remember, I think its in Physical Review B.

M: No, it's in Physical Review Letters.

Oh, maybe it did finally get there. Eddy Cohen maybe was the reviewer. Of course Eddy Cohen was a little jealous you know, - you don't want to get into that. I must say I sympathize with Eddy, he was so close, and only had to make the final jump. But we had to come to it from a completely different point of view, which emerged in an unbelievably simple way. Let me say one other thing which I keep saying at conferences when I get the chance. The significance is not the long-time tail. The significance is that hydrodynamics applies at the microscopic scale. This is the real philosophical break through. I mean when you listened to Uhlenbeck in those days, he would say that the kinetic time of a collision which for hard spheres is the time between collisions, and is 10^{-14} seconds, and there is the hydrodynamic time scale, which is seconds. I don't know what people imagined between 10^{-14} and seconds, but the big push philosophically, is that hydrodynamics applies on almost the kinetic time scale, that is it merges with the kinetic time scale. And from what I can remember historically, that dates back to an argument between Boltzmann and Mach. Mach, of course, did not believe in kinetic and molecular theory, and Boltzmann did. Mach was, of course, a great hydrodynamicist, but did not believe there was any connection. That break between kinetic theory and continuum hydrodynamics was deeply inbred in every statistical mechanician. That, to me, is the real importance. Once you realize that hydrodynamics applies to a molecule moving in a fluid, its obvious that you get this long-time tail. Nobody dared believe that until we did the computer experiments.

M: At the same time, I don't think there has been an experimental check of long-time tails.

People have taken colloidal particles, as small as they can make them, and they do find the tail.

M: But there still macroscopic objects.

Or mesoscopic. There is an interesting neutron diffraction experiment which you may not know about, done in Grenoble. It took two theses to find evidence for the long-time tail. You see you can't do it for high density fluids because the back scattering dominates, so they took, I think, alkali metals, either sodium or potassium at elevated temperatures which is a fairly dilute liquid, and studied the dynamical structure factor, $S(k, w)$. And they found the tail after two PhD theses on a real microscopic scale, that their data was at least consistent with a long-time tail. I don't think they could be sure that their was a long-time tail, but their data was certainly consistent with one.

M: So when you found the long-time tails for the velocity- velocity correlation function, you immediately thought that this would be the same for every other transport coefficient ?

Right, for the kinetic part, but not the potential. So you have to go to very low densities because otherwise the potential part, say for the stress-stress correlation function, starts to dominate even at intermediate densities. So we could never go to sufficiently low densities to see the tail in the kinetic part of the viscosity. We just didn't have enough "umph". That's where the cellular automata people came in. There's a Kadanoff thesis, and a piece of work by Frenkel where with cellular automata you are able to go to much lower densities, with much higher resolution. Cellular automata runs many orders of magnitude faster than molecular dynamics, and Kadanoff and a student,Guy Mac Namara who eventually became my postdoc, saw not only the tail in the kinetic part of the stress-stress correlation function, but also a correction to the coefficient A in $A\log(t)$ which we had predicted through a two line self-consistency argument. You see, the coefficient $|A|$ depends on the viscosity which diverges also, and our argument said that it should go as the square root of $\log(t)$ instead of $\log(t)$. In fact, a student of Irwin Oppenheimer in a huge Phd thesis found analytically the square root log dependence before Frenkel, who found it by cellular automota. So we predicted this from the beginning through a hand-waving argument, which took two thesis, one analytic, the other numerical, to verify.

M: Now the long-time tails is from 1962 to 1968 roughly ?

Well, I would say 1965 to 1968.

M: Ok, and now you refer to the work of Daan Frenkel which is in the 1990's, so it is more than twenty years later. In between, the long-time tail paper you published had an enormous impact. Several theoreticians tried to get the long-time tail through many analysis. How do you see that ?

Well, after ten years on equilibrium, we spent ten years on transport. We did not only the diffusion, but also the viscosity. We looked for tails there. You know sometime in that ten year period there came non-equilibrium statistical mechanics à la Hoover, and there was a lot of comparison between non-equilibrium statistical mechanics, and our fluctuation - dissipation calculations. We never entered that because non-equilibrium statistical mechanics has this boundary problem which vastly affects the results. But to see any results, they have huge stresses and strains on the system in non-equilibrium statistical mechanics, and of course our fluctuation - dissipation results were in the zero gradient limit, so there was the question of how to extrapolate to this limit. Our argument was that the viscosity would be the same calculating it in the two different ways. My view is that the expansions in the gradients doesn't exist either, because even in three dimensions the non-linear Burnett coefficients diverge. It took us a long time to show that. To work out the correct Burnett coefficients, you have to introduce some memory function to the definition of the diffusion coefficient. It's very complex, we only did it for the Lorenz gas. After it got so complicated, I gave up, and nobody has calculated the higher order gradient corrections beyond Navier-Stokes, even for three dimensions, except we did it for the Lorenz gas. Anyway, that took us ten years. And then I said, enough of that, and started to go into quantum many body problems.

M: Before going into quantum, let me say that you have with your paper made a revolution for a community that was ready for it, in the sense that people were smelling that there was something wrong in the picture of transport, and you came with your paper, and this was a kind of evidence that would cause everyone to jump into the problem. You provoked a lot of computations. At the same time, at the end, you come with the cellular automata evidence of this $log(t)/t$, and the theoreticians have left the field.

Yes, that was solved.

M: No, it's not solved, they simply escaped. You said that no one has calculated the Burnett, or this Super-Burnett , you said that all these computations are extremely complicated. They left, and went to other fields. So you killed the field.

Yes and No. I think we did the easy thing, and it's now very hard to go further. You see I don't think we could solve the Burnett problem, I mean the higher order gradient corrections. This is why we are going back to these hybrid methods. You see, we are now returning after this quantum hiatus, back to transport. But whenever we are in a non-linear regime, we will just use particles instead of hydrodynamics. We will only use Navier Stokes only when it is rigorously justified, when the gradients are small. And when they are not small, I think the only way to escape is to use particles. Its like the virial coefficients. You can calculate a few, and if that doesn't do, you give up. In the transport case, even the first one gives you difficulties to correct, so you just give up, and just use molecular dynamics. That's my rationale of giving up. It takes another generation of computers to do the hybrid particle mesh method.

M: Was that something you had in mind to do from the beginning, to do non-linear hydrodynamics, and go beyond Navier Stokes ?

Well, you know sometimes it is good to leave a field and see what boils up, and nothing boiled up. It now becomes fashionable, because people want to do mesoscopic instead of microscopic problems, small clusters or whatever, to extend any of these methods to longer length and time scales. So the hybrid approach became the natural thing to do.

M: OK, now during that time, the sixties, and late seventies, it was a time of incredible growth for molecular dynamics. I remember the report of the first CECAM workshop, on the simulation by molecular dynamics and Monte Carlo simulation of water, of Rahman and Berendsen and people like this. They would show you all the possibilities offered by the method, polymers, chemical reactions, proteins, biology, much of what has been achieved in the last years, and is being worked on now. During that time you still concentrate on problems which are more fundamental. So you have put the methodology on firm grounds, and you have not gone along with it. You left it to others.

That's precisely why I went into quantum mechanics, because it was clear to me that you never would do water well, with pair or triple potentials, it's always an artifact. I mean it's sort of a numerical fitting job. You try to get a potential which would fit the properties of water. But it's never an a priori theory where you predict things reliably. You can dream up potentials, and reproduce some of the properties of water, but not all with these potentials. I said, by Jove, the potential is the limiting factor. We had better do something about getting the potential right. People don't realize that we already knew, for example for argon, that you can try to get a really good pair potential from low density data, treating equilibrium properties and transport coefficients, and fit the scattering experiments, and make everything consistent. If you then go to high densities with that potential, and it differs by twenty percent from the many body pair-potential properties even for argon. So if that doesn't work, you'd better do something about the potential. I always was interested in quantum mechanics, but at that moment I decided that was the limiting thing, and to see if we can do water, which I predicted would require one hundred protons, fifty oxygen nuclei and a thousand electrons. That was a big job, and still is if course. So we went into quantum Monte Carlo.

M: So the first person you collaborated with was David Ceperley ?

No, it goes way back to Steven Brush. He was one of those extremely promising people, Rhodes scholar, Westinghouse fellow, all that good stuff, and he had worked on functional integration, that was the way to do quantum mechanics limit, that didn't work out. He came post-docing with me, and we started out on the pure repulsive Coulomb potential, that's the only other potential that I've worked on aside from hard spheres. I got him started working on Coulomb potentials. It's an interesting story in its own right. We were interested in the interior of the sun, whether the protons in a uniform electron backround would form a solid-fluid phase like the purely repulsive hard-spheres potential. Well, it turns out that the centre of the sun is nearly a perfect gas, so it was crazy to think that it might be a solid. Anyway, that resulted in the first paper on the repulsive Coulombic potential by Brush, Sahlin and Teller showing the phase transition. I had left on sabbatical, although I started him Brush the problem. This was in the early sixties.

M: You were visiting Orsay ?

No, let me see. My first sabbatical was the Guggenheim to Cambridge and Leiden, and this second one was to Israel and Rome. I worked with Shneior Lifson, and in Rome with Careri. It was one of those sabbaticals when you just want to get away and find interesting places to go to. To go back to Brush, he just wasn't a creative physicist. He decided he couldn't be an Einstein, and therefore he wasn't going to be a creative physicist, and became an historian of physics. Then I had Kalos out for two summers. I knew that Kalos was working on the quantum Monte Carlo problem. I sat next to him every day, it must have been the sixties, I really tried to understand his algorithm, but it was so complicated, and he could not explain it to me. I met Ceperley in Corsica at a summer school. I was very impressed with him. He was a Kalos student. What happened then is they formed a chemistry centre here on the hill, at LBL, and they made Bill Lester head of it. They were able to hire a bunch of theoretical chemists, and I persuaded Bill Lester to hire Ceperley and also Peter Reynolds, and they both have made major contributions to quantum Monte Carlo. But as soon as Ceperley went there I had him coming over to Livermore, so we started working together from then. The chemistry centre on the hill collapsed after two or three years, and Ceperley transfered out to Livermore. Quantum Monte Carlo was made clear to me by Ceperley. Well, to be fair to Kalos, quantum Monte Carlo had progressed a lot by then, and was much clearer. Anyway, Ceperley had a clear understanding of quantum Monte Carlo, and we started talking. He had worked on the electron gas, by an approximate method, variational Monte Carlo. I said, David, no one is going to believe your results, unless we do it exactly, without approximation. That's how we got started in the electron gas , and we did it exactly eventually. It took thousands of hours of the fastest (Cray 1) computer. We just bullied our way through, both intellectually, and numerically, and we got a classic paper, the most important paper in condensed matter physics at the time. It may still be. Someone told me that it rivals the original Walter Kohn paper for citations. It was a very nice job, and David was certainly the intellectual driving force behind it.

M: When you came to consider the quantum problems, were you driven by intuition that you got from studying the hard sphere system ?

No, they were totally disconnected.

M: But you never had worked on quantum problems before.

Well, I had never done anything worthwhile to say.

M: So you never solved the Schroedinger equation numerically.

No, I had never worked in quantum chemistry before. You see, the one thing that carries over is Monte Carlo. I mean I saw that in quantum chemistry they never got sufficient accuracy, and always ended up guessing, or extrapolating to an answer. I knew that density functional theory was a dead end. It's a mean-field theory, and you can't go around that. So the only thing that came over from classical physics, is that Monte Carlo can solve the many body problem rigorously. So I knew that we had to go high dimensions, it's a many body problem. That was the first basic thing that pushed me to quantum Monte Carlo. So then you look what is the status of quantum Monte Carlo. When Ceperley and I came into the problem, the variational method had been developed, and diffusion Monte Carlo had been developed, basically by Kalos. You see, the mathematicians had a huge problem at first. You know that Mark Kac had done diffusion Monte Carlo in 1949 ?

M: He computed the ground state of the hydrogen atom.

Yes, but he could never get enough statistics because he didn't have an importance function. The idea was that when the electron wandered close to the nucleus, the system just tried to build up the Coulomb singularity, and of course he never got enough statistics. So while the mathematicians were scratching their heads, Kalos introduced this importance function. Kalos really solved the Boson problem by diffusion Monte Carlo, or Greens function, which is much the same. But the fermion problem was still there, and of course, it still is there. We argued that the fixed node ought to be a pretty good approximation because the wave function is small there, and it is a good approximation. But you need such a high accuracy in the quantum many-body problem, because what matters is what the outer electrons do, that even the fixed node approximation is not good enough. It's no better than density functional theory, or quantum chemistry, it gives you a one or two kilo-calorie error for most chemical molecules. So we did fixed node, and then release node, and then we found this numerical instability which we are still trying to work out.

M: So that's the early eighties.

Yes, and then I must have spent ten years exploring various aspects of the problem. The chemists had problems with the H2 + H barrier, Zare had done some experiments which disagreed with theory, and we thought that the potential barrier calculations might have been at fault. It turns out that the chemists had got it right, but we got it confirmed rigorously. We had already done a bunch of problems just to explore the accuracy of the fixed node approximations. Ceperley had checked the stability of the release node for hydrogen while looking for its metallic phase. There it is barely stable, and as you go to higher Z elements, you have problems. So we have to make the release node more widely stable, its the only way to go, that's what Kalos is working on. See, we did finally get back to the inter-molecular potential of two helium atoms. We got it right to one part to the tenth, which is by far the highest accuracy yet. It's a four electrons problem, this interaction potential is the equivalent of a Lennard Jones potential. One of the problems I would still like to do is three helium atoms, which is a six electrons problem, and get for the first time a three body force. It's never been done right, except for the Axelrod Teller asymptotic form. The point is that for small systems, you can overcome the sign problem of the instability, because for small systems, you can control the exploding number of positive and negative walkers by canceling them. So we have been doing this exploratory work for ten years, what you can do with fixed node, release node and small systems with cancellation of walkers. We now are, or rather Kalos is, in a position to control the exploding population in the release mechanism. He's got some results on a six electrons problem, but it’s still inefficient. Not only do you need stability, but you also have to get an efficient method. It’s a highly technical problem, but once it is solved, it will make an enormous difference to chemistry and material science. We certainly have every expectation that quantum Monte Carlo will eventually succeed.

M: Ceperley was at Livermore during that decade of collaboration ?

Well, for the first two or three years he was part-time, as he was also in Berkeley, and then he became a staff-member at Livermore, after that he left for an academic position.

M: Was there anyone else that you would like to mention in this quantum Monte Carlo work ?

Yes, Pollock, and Reynolds at the beginning. We wrote a paper with Reynolds and Lester. Reynolds was a pretty influential intellectual force. I think we did work on fixed node with Reynolds, and the paper includes Reynolds, Lester, Ceperley, and myself. The Green function release node electron gas I did with Ceperley. And then Ceperley and Pollock, with me standing on the side-lines, did the finite temperature quantum Monte Carlo problem, making the Feynman path integrals efficient. That was a very successful collaboration between Ceperley and Pollock, where I just gave advice. They made the Feynman path problem for helium practical. That’s a technical problem of how to move the polymers efficiently. As you know that’s a mapping of the Feynman path problem to a polymer problem. To move these polymers efficiently was quite ingenious.

M: You didn’t say anything yet about your collaboration with Charlie Bennett, can you say a bit ?

Well, I’m not sure how it happened, either Turnbull sent him, or more likely he wanted to come himself. He was a graduate student at Harvard working with David Turnbull, you probably have heard of him. So he appeared after his candidacy exam at Harvard, and then spent all his time at Livermore.

M: As a postdoc ?

No, as a graduate student, that was his Phd thesis. He came driven by a problem.

M: That’s is your first Phd student that you are talking about ?

No, I had Ed Alley, and I had a number of Phd students through the department of applied science, which is a branch of the University of California at Davis, and is located at Livermore. I taught there for a while, and I had a bunch of students there. Ed Alley was probably the only really successful student that I had through that, and he worked with me on transport.

M: Generalized hydrodynamics ?

Yeah, Sidney Yip visited us, and we worked on generalized hydrodynamics, that was a very nice piece of work, that was part of his thesis.

M: That was the early eighties ?

It was earlier than that, it was in the transport phase, before the quantum problem. He worked with me for close on ten years, and maybe eight years to get his thesis. We did some very nice work on the boundary condition, for Stokes law. The first problem we did was a hydrodynamic calculation to know what size and mass you need for a particle before you approach the Stokes limit. You know there is also this issue of what boundary conditions to use, slip or stick. Generalized hydrodynamics was another very good problem that we worked on. He was a very good guy, he's still at Livermore. Let's see, we got diverted.

M: Yes, we were talking about Bennet.

Yes, you see Harvard has a system that after you achieve candidacy, you can work with anyone you like, so he came to me. He came to me with an isotope problem, the isotope problem for diffusion in a solid. You have a vacancy in a solid, and a particle jumps into the vacancy. Is there a correlation of that jump with the next jump of the particle, because if there is a correlation, the existing theory for isotopes was wrong, because they assume that all jumps were un-correlated, but successive jumps could be correlated, and in fact that's what we calculated. In the process, of course, we had to develop this rare event algorithm. It was clear that we couldn't wait for a particle to jump into the vacancy, it would take much too long, so we had to do something about that. So he came with the problem, and then we found an algorithm to solve it, namely this adiabatic rare event algorithm which everybody now uses, where we force the particle to the top of the barrier. Of course in this case we knew where the barrier was.

M: You knew the reaction co-ordinate ?

Yes, we knew the reaction co-ordinate, physically we knew it, and that's of course still the big problem. People don't know that barrier generally. So we forced the particle (hard spheres again), that is the reactive one, the one that was going to jump into the vacancy, and calculated the work it took from the pressure difference on both sides of the confining walls, until it got to the top of the barrier. We got the transmission coefficient, because we didn't know exactly where the top of the barrier was, so it was necessary to see how often it would fall back, and how often it would fall in. That's the adiabatic rare event reaction path mechanism, which Bennet and I wrote for the first time. I don't know, did Andersen have it at the same time ? Anyway we certainly developed it independently. He was an extremely bright student, very deep. He was a sort of a hippy.

M: Do you remember the years ?

It was the hippy years, late sixties, early seventies.

M: So during the Vietnam war ?

Yeah, he had long hair and so on. I was surprised that IBM hired him.

M: You were very conservative.

Ohhh, I was never conservative.

M: And you still are !

No, well I am conservative in some ways, politically mostly conservative, but in science I am not, I am a radical rabble rouser in science, that's for sure.

M: So during these years Bennet was a hippy.

Yeah, and IBM hired him, despite the fact that in those days in IBM, you had to go to work in a coat and a tie if you were a researcher. But they recognised his talent. He had these two phases- a statistical mechanics phase, and a mathematical phase. He was really a mathematician type, and as you know, he is really one of the leading lights in quantum computing now at IBM. Actually, they thought he was distinguished enough to make him an IBM fellow, which is a rare distinction. But he hasn't really pursued this statistical mechanics interests which we did. He was driven by a problem, and we found an algorithm to solve it.

M: He also developed this method to compute free energies.

Wait a moment, I worked with David Young on that as well. We were trying to find if in equilibrium FCC or HPC was more stable for hard spheres. It was certainly a problem which we never solved, or at least not very well. We did to some extent solve it by making an expansion around the close packed limit. I think I did that with Zeni Salsburg. We calculated the first correction term in the expansion, and I think we found that FCC was more stable, but barely. There was a very small difference in free energy. Bennet may have used a different method for other problems.

M: He developed a method which is quite general to compute differences in free energy.

Is that a method based on using harmonic oscillators in some limit ?

M: No, it's a method using overlapping distributions.

Is that umbrella sampling ?

M: No, but it's related.

He may have done that independently, we did develop a fee energy difference method, but not that one.

M: OK, so with Bennett you really calculated the chemical rate constant ?

That's right. We got the chemical rate constant, which is a key paper.

M: Yes, because it allows calculation of the diffusion in solids.

Yes, but now it can be applied to any rare event, which is too slow to follow or wait for with molecular dynamics.

M: OK, so this was Charlie Bennett the hippie.

Well, I brought him to my house so that we could work, I remember all sorts of interesting discussions.

M: At some time in your career at Livermore, you were also head of an experimental group. Can you say a bit about that ?

Well, I don't know quite how this happened, it was for a very short period of time. When I first came to Livermore I was a consultant on the equation of state. I was a one man equation of state guy for Livermore. For material problems, they needed equations of state at high temperatures and pressures, so I learned all the techniques. When I came back from the Guggenheim fellowship, somehow Christiansen was getting his Phd, I think with Edward Teller, in the shock explosive programme. I think he had come to Livermore through Los Alamos. Anyway, he was part of the experimental equation of state group, and I started working with him, and we did some very pioneering experiments on high pressure: when things go into the metallic phase, how quickly chemical reactions take place, or crystal structure changes. Actually, we shocked the alkali halides for very high pressures. I was sort of his thesis supervisor. Then we expanded into more interesting experiments. Could we turn carbon into diamonds. We did indeed do that, and we ruined one of Harold Uri's great theories. You know when they found diamonds in meteorites, they thought that the only way that those diamonds could be produced was by the break up of a large asteroid, a comet or whatever, because you needed, people thought, very high pressures and temperatures at the interior to make diamonds. But it turned out you could make diamonds in a meteorite through impact, because of the shock wave, which people hadn't thought of. We did the experiment, and found diamonds. And so I became an expert on shock waves. I used to give a talk, a millionaire for a microsecond, because thats how long the diamonds lasted. Anyway, we did those carbon experiments. We also turned iodine and phosphorous metallic. It was also the origin of the first shocking experiment of hydrogen, which turned out to be a very important equation of state for nuclear weapons. I actually designed the experiments. Somehow, I became more and more in charge of this explosive group. It was a big group, and I was there for a very short time because it became so time consuming, to worry about what engineers were going to get what screw and where, that I decided that this was just not what I wanted to do.

M: When was this ?

This may have been in the late fifties, rather early on in Livermore.

M: Before the long-time tails.

Yes, I would say so. It was mostly equation of state. Hard spheres are also relevant to equations of state at high temperatures and pressures.

M: Were you considering leaving simulations to move to experiments ?

Oh no, it was clear that experiments were not my cup of tea, I knew that early on in my chemistry career when I broke all the test-tubes in organic chemistry, or whatever chemical experiment. And these explosive experiments take a lot of care. So I had a lot of other people that helped me run the experiment, so I was more a supervisor. But I was interested enough in the results of the experiments, because they were relevant to theoretical work.

M: So it's from that time that you got to like, and have so much knowledge about shock waves.

Yeah, basically I supervised the thesis of Russ Christiansen, and did some very interesting experiments, so I got very knowledgeable about shock waves.

M: Brad Holian came much later, in the late seventies ?

Yes, he was a graduate student in the chemistry department in Berkeley with Bill Gwinn who was an old friend of mine. I talked to Bill Gwinn a lot about computerising physical chemistry courses, doing computer experiments. He was an extremely bright professor, a pioneer in a lot of microwave work, a very nice and very bright guy. Anyway, he had this graduate student. I don't know how exactly it got going, but Gwin had an interesting theoretical problem which was about a phase diagram for the crystal structure of helium. You know, that of all the rare gases are FCC, except for helium which is HCP. I had previously worked on a problem with someone called Carter. Anyway, we showed from general principles that the hexagonal phase had to have lower energy, for hard spheres again. It had a lower zero point energy than FCC, and that had to do with the number of nodes in the wave-function and the symmetry of the crystal. We actually calculated the energy difference between FCC and HCP for hard spheres, and it incredibly matched the known difference in energy between the two crystal structures. It was incredible that such a simple model could do that well. Anyway Gwinn had a similar problem but with a Lennard Jones potential. I've forgotten exactly the origin of this problem. Brad Holian was working on that. It had to do with a similar problem,, so it was basically the same problem. We worked out the the energy difference between FCC and HCP using Lennard Jones instead of hard spheres. Thats how I got working with Brad. I introduced him to Monte Carlo, and molecular dynamics. Then I persuaded Bill Wood to hire him as a postdoc.

M: He started his postdoc on shock-waves ?

No, I don't think he worked on shock-waves while he was here. He only got involved with Bill Hoover in Livermore. I don't think he did anything on shock waves. We did some intricate quantum problems. These were zero point energy calculations for a one particle problem in a box with very complicated boundary conditions. That's not Monte Carlo, but purely numerical using normal mode analysis. He did not do any work on quantum or classical Monte Carlo with me. I had connections with Los Alamos, and recommended that he go there.

M: The question in my mind was the shock wave.

Yeah, but there is no connection between Brad and me on shock waves. He picked that up in

Los Alamos. But shock wave work is pervasive in Livermore and Los Alamos. That's one of the major experimental pieces of work that's being done.

M: So despite your experience in the shock-wave experiments, you were not the driving element in developing shock wave simulations ?

No, Hoover was. I didn't think one could learn much from shock wave simulations, except that hydrodynamics works pretty well there, but I knew that already. So it is a little bit messy, and I am not sure what there is to be learned in simulating shock waves. Now, I think Holian does much more complicated shock wave computer experiments, seeing how crystal structure shifts and so on, but it's not my cup of tea. I am happy to have him do that. These are massive billion atoms simulations of shock waves. It's just brute force from my point of view, but it's very interesting.

M: And your view on non-equilibrium molecular dynamics. You said something on it which was that it was competing with the formulation that you developed for the transport coefficients. Retrospectively, how do you see this competition ?

If you want to do linear transport coefficients, fluctuation-dissipation is the only way to go. Non-equilibrium molecular dynamics has to do with strong gradients, and I am suspicious of strong gradient results. In terms of extracting transport coefficients, the boundary conditions really are very perturbing on the calculation, so if you want to do non-linear transport, I believe that this hybrid method is a much better way to go.

M: OK, so what you say, is to compete with near equilibrium properties, it's no good, but it can be used to investigate non-linear transport.

Yes, but with a little danger because of the boundary conditions. The gradients are much stronger than in any experiment, because in order to get any signal out, you have to make the external gradients so strong that it's dangerous, and is not, I would say, a very elegant way to simulate non-equilibrium processes. But it's being used a lot.

M: Yes. and as a matter of fact, we have talked a lot about several periods of your career, and now we come to the last period, which maybe started in the late eighties with the simulation of lattice Boltzmann with Guy Mac Namara, and DSMC simulations with Alex Garcia, these hybrid methods with Hadji Constantinou, and so on. I mean, this last period is really devoted to non-equilibrium problems, right ?

Yes, what we're after are hydrodynamic instabilities.

M: A natural question which comes is, you've been the promoter of molecular dynamics, but for these problems you leave molecular dynamics somehow to go to methods which are not phenomenological, but somehow are less rigorously founded or based.

Well, let me explain this to you. I call lattice gas and lattice Boltzmann, poor man's molecular dynamics. It's a way to do molecular dynamics cheap. The basic problem is that even molecular dynamics has its limitations right, that is for big systems and very long times.

The lattice Boltzmann excursion was an attempt to see whether one could do by cellular automata very big systems and for long times. That, unfortunately, ultimately failed. But there was a four or five year hiatus before I decided that. We really tried hard. It's an approximate method, but only in the sense that it crudely integrates particles dynamics. It's still in principle a more efficient molecular dynamics, but it failed. Now, the excursion into the Boltzmann equation, into DSMC, well, DSMC is an exact method to solve the Boltzmann equation, however the Boltzmann equation has of course molecular chaos in it, and therefore is inexact, because even at low densities you have this long time tail. You have a very legitimate question, why are we piddling around with an approximate Boltzmann equation. Again, it's an effort to do molecular dynamics much faster. DSMC is a method which is 10^5 to 10^6 times faster than molecular dynamics. And the key point is that for hydrodynamic phenomena, which is what we are after, those ignored correlations don't matter. I would be highly surprised if, whether a transport coefficient has a long time tail or not, matters. For hydrodynamic all that really comes in is the transport coefficients - whether you have it off by a few percent should not matter whether you develop the instability. So, I am going into DSMC simulations of the Boltzmann equation coupled to Navier Stokes, because DSMC has the non-linear effects correct, has the fluctuations correct. It doesn't have the correlations correct, but that probably doesn't matter. DSMC is a much cheaper way to couple to continuum methods than M.D. We would love to couple it to M.D, we are going to couple it, but it's 10**5 times slower, and therefore, even if we know how to couple it, it's so slow, that the MD section takes all the time in a hybrid scheme, and therefore we don't want to do it. So, I am forced to use the Boltzmann equation, which is not a bad approximation, that's what my claim is, particularly for hydrodynamics. Because, the same phenomena occur in a gas as in a fluid, I mean instabilities and so on, so I think we can get away with using the Boltzmann equation, that's my rationale, you may not accept it.

M: When you got the Boltzmann medal, you presented a path going from the hard sphere liquid transition to solid, and ending with the DSMC simulation and the hybrid method, and somehow I think you were given the Boltzmann medal because you have given the community a method which has been so powerful, and pervasive. Picking the right problem at the right time.

Let me rationalize this. We did find by molecular dynamics the corrections to the Boltzmann equation, and in fact we also made some vast improvements to DSMC with Alex Garcia and Frank Alexander, making it consistent and extending its accuracy and so on. I did talk about the validity of the Boltzmann equation, and after all it is Boltzmann that the medal is named after, so I felt obliged to talk about what we had done to the Boltzmann equation, at least half the time. I didn't think I should just talk about molecular dynamics, but only so far as it showed that even at low densities Boltzmann is only valid in the asymptotic limit. I wanted to talk about what had happened to the Boltzmann equation itself. So that was my rationale for not just talking about molecular dynamics.

M: Now coming to the Boltzmann medal that you received, how do you see that ?

Well, I think there are two things to say of it. One is that it's great to receive it. And I think what it really means is that numerical methods have become accepted even by the statistical mechanical community which is very analytically and theoretically oriented. So, I think that's a big break through, that numerical methods are being recognised as a legitimate intellectual activity in the theoretical statistical physics community. The second thing, is that in all modesty, I think we have really made important contributions to transport and Boltzmann through numerical methods. I think if you look at the improvements of the Boltzmann equation since Boltzmann, the major improvements have been through numerical techniques. Calculating transport coefficients at high densities, applying the fluctuation-dissipation theorem, finding the long time tails, that the Stossansatz for molecular chaos is not valid, those are really deep, major contributions, so I think it's both recognising the method and the results, which is great.

M: Sure, but as you said, the community was very mathematically oriented. The first few Boltzmann medals were given, one can say, for proving theorems. Now M.D. is being accepted because it's a very practical tool in computing material properties, in predicting behaviour and so on. You see this invasion of the methods into the fields, without being involved. How have you kept yourself at a fundamental level ?

I think if you look to the fundamental contributions that computers have made to physics, not just to statistical physics, the long time tail is one of the few examples where computer experiments have had a fundamental impact. I think that is being recognised. The applications are incredible, I would have never predicted the pervasiveness of molecular dynamics and Monte Carlo, and they are great and they are useful, but I think the thing that the statistical physics community appreciates the most is the fundamental contribution the method can make to statistical physics. So I have sort of stayed away from the applied, because there are so many applications that I can't possibly compete in my small scale operation against these groups that have these massive application calculations. So I just stick to my little toy fundamental problems.

M: We have covered almost sixty years of science, and the development of a new method. What kind of advice would you give to a young man. I mean, what important problems need to be solved ?

Through molecular dynamics and Monte Carlo simulation ?

M: Yes, but not exclusively.

Well, obviously, there are two big problems left, maybe three in computational physics. I have tried to piddle with one of them, which is the sign problem. I leave it in the capable hand of Kalos to solve. There are ways to go about it, they may not work, but he's got to keep trying. That will be a revolution, once quantum Monte Carlo becomes as cheap as classical many body dynamics. It will revolutionize chemistry and condensed matter physics. The other big problem which has been around for seventy or eighty years without much progress, is turbulence, right ? Both problems look very difficult, but the hybrid approach might make some headway on the instabilities. The idea is not to guess how long wave-length energies cascade down to short range ones, but to start at short wavelengths, and see how the long wavelength ones build up, that's the idea. How do the local molecular fluctuations lead to coherent long range instabilities. Somehow, macroscopically, some vortex develops at the boundary from microscopic fluctuations. Those are two good problems to work on, I only have one good technique, these hybrid techniques at the moment, to see if the boundaries matter - we are making progress on it. The other problem which is outside of statistical physics, is pattern recognition, this is a computational physics problem now, which computers are very bad at, which I used to work on, modeling the eye. It has to do with some missiles coming at you, that's part of star wars. They just rise above the horizon against a very noisy background. How do you recognize a coherent signal in a noisy background. A frog can do this very easily. It sits there at night, at dusk, not moving his eyes, sticks its tongue out as a fly goes by, and catches it. How does he do that ? The computers are incredibly stupid at this. Anyway, we've modeled the eye, we've built an analogue computer, we've modeled the eye of a frog - it's sort of fun, but it's still at a very primitive stage. Pattern recognition is a very deep scientific problem. There are many other problems, but those are the three that I think a young man could well spend a few years making some progress on.

M: We see in these last forty years, the science community has increased a lot. We have far more people working all over the world, and so on. Do you see any encouragement to attack the fundamental problems or is it getting more and more applied ?

It's more and more applied, but sometimes the very best way to work on a fundamental problem, is to work on an applied problem, like on the isotope problem I mentioned; you think about a problem in a very different way. Many of the fundamental problems arose while trying to understand an applied problem. So if people keep their eyes open, not just narrowly focused on finding some particular applied use, then you can discover some pretty fundamental things. These discoveries are really haphazard. You play around, you just study the velocity correlation function, but you have to be aware that there is something strange happening, when you see the long-time tail. Then you suddenly discover yourself making a rather fundamental contribution in transport theory.

M: It's quite similar to your career, you have always been in an environment which was linked to great laboratories, where they were developing very applied things like the atomic bomb and so on, and you always stuck to fundamental problems.

Yes, but you see in a government lab you have a whole range of people with different talents. You do have this in academic communities as well, but they are all isolated. I mean, you talk to astrophysicists, for example. I have worried about the interior of stars, the interior of the Earth, you know, there are people around who bring you these problems, and you talk to them. I guess there are very bright people, who are more willing to cooperate than in the academic community, because they are not so bent on their own career. They are sort of more bent on problem solving. It's easier to collaborate with them. There are some very talented people. Sometimes you have to hire them yourself, of course, but they are very diverse, so you have a very stimulating atmosphere, more so than in the academic world. It used not to be true in the early forties you know. There were only a few theoretical physicists, and everybody talked. But lately everybody has got very narrow into their own specialty, their own empire, their own grants, their own little problems, so it's much harder to work with them.

M: So was this a sort of heritage from the war, when they developed the Manhattan project ? They hired some very good people.

Superb people ! They are disappearing quickly, and the quality of people in the government labs is going way down, and the applied pressures, and the bureaucracy is going way up. The atmosphere has changed enormously. I doubt that I could have the same career now in the lab. I mean then, as long as you did something relatively relevant, they let you go, and you just did your thing. Now, everything is much more controlled. Many of the good people left over from the postwar period are retiring, so it's hard to get good people to come into the game now.

M: Did you interact with Edward Teller ?

Well, that's a complicated problem. He's very hard to interact with unless you enter his frame of mind. He sort of treats you like a flunky, and I didn't particularly enjoy that status, so I didn't interact with him so much. I talked to him about things, of course, during the early days of Monte Carlo, and I see him off and on, but I had no real scientific interaction with him. He's extremely bright, extremely sharp, very stimulating, but you have to sort of enter his intellectual game, which wasn't my cup of tea.

M: You have children right ? We started the interview with your father and your brothers, but you have children.

Yes.

M: Are they scientists ?

Yes, one of them, the girl is a neuro-biologist.

M: Doing research ?

Yes, at Rutgers university. But she's more a housewife than she's a scientist. She has two small children, and her career is less important to her than her family.

M: And you have one boy ?

Two boys. One started off as a physicist at Harvard, but did a minimum amount of physics, it wasn't his cup of tea, and then switched to the history of science, and has now a very successful career in the history of science and technology. He's now a professor at Northwestern. The second son started off in biology at Stanford, again my urging him to do something scientific and practical. He was clearly not meant to be either a theorist, or an experimentalist, and is now a rabbi in New York. After finishing biology at Stanford, he went to a Jewish theological seminary in New York for some seven years, and is now a very successful rabbi in Manhattan.

M: A successful rabbi ?

Yes, he has a congregation of his own at a rather tender age, and seems to be very popular and successful.

M: So that will lead me very naturally to the last question. You know the questionnaire of Bernard Pivot ?

Who ?

M: Bernard Pivot, he's French, and interviews novelists, and he always has a questionnaire at the end. One of these questions I will ask you, because it's funny, but don't take it seriously. If God exists, what would you like him to tell you when you arrive up there ?

Oh, you mean what problem would you like him to resolve for you, you mean on a technical scale ?

M: No, not at all. Anything.

Well, I would really like to know if the universe will collapse again to a big bang. You know that everybody seems to think now that the universe will continuously expand right ? It's a flat universe and so on. But I somehow believe that from the big bang, we're still in an accelerating expanding phase, and I think that there is some estimate that after some eighty billion years, the universe will collapse again, and I wonder if that's true. I will never find out in my lifetime whether its true, so I have to ask God that question.