

SIR JOHN POPLÉ Ph.D.

ORAL HISTORY

COMPUTERWORLD HONORS PROGRAM INTERNATIONAL ARCHIVES

**Transcript of a Video History Interview with
John Pople
Professor, Department of Chemistry
Northwestern University**

**Recipient of the 1998 SGI Cray Leadership Award for
Breakthrough Science**

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DSM: Today is March 26, 1998. We're interviewing Dr. John Pople who will, on June 8th of this year, receive the 1998 SGI Cray Leadership Award for breakthrough science. This interview is part of the personal research collection held by the Smithsonian Institution's National Museum of American History. Unless otherwise noted it will part of the public record and available for use by scholars and the public subject to the normal Smithsonian Institution restrictions.

We can stop this interview at any point, and you can indicate portions that you would like to have embargoed for up to 25 years. If there are questions that you would like for us to ask, again stop the interview; feel perfectly free to do that. We're not trying to do a television program. We'd loved to have suggestions for things that we might not otherwise know to ask.

I'd like to begin at the beginning. Tell us when and where you were born and where you grew up?

JP: I was born in a small town in the West of England. A place called Burnham-on-Sea, which is a small town with a population of about 5,000. My father was the owner of a retail clothing store in this town. The town was a seaside resort. Some of the people there made a living out of accommodating tourists. There were some people who were independently wealthy there.

A number of people lived in a town like that were colonial servants that were back on leave from India. Some people had to leave their families in this town. The husband went out to work in the colonies and aside from visits, left his wife and children behind. So, it was a small community.

My father, as I said, was the local men's clothing retailer. He was good at the job, so we weren't particularly hard up. Nobody was rich as this was during the depression, of course, when I was a young child. However, there was a rather rigid class structure in the town, which had some effect on what happened to me.

This had to do with the school that I went to. In that part of Britain at that time there was a distinction between people in the upper middle class and the lower middle class, to which my family belonged. As a result there was some difficulty about getting into a good school.

There was in fact, a very good preparatory school in this town, which was attended by some of the local children. But they did not allow the children of people in retail trade to attend this school. So as young boys, my brother and I went to a rather inferior school. This evidently dissatisfied my parents significantly. They were ambitious for our future.

My father frequently said, "When you grow up you're not going to stay in this town. You'll have to go into the outside world. You have no future in this environment." So, at the age of 10 they made arrangements for me to go to the school in Bristol, which is the largest city nearby. I was sent to the preparatory part of Bristol Grammar School.

Now, grammar school in England, unlike this country, means generally superior high school. Bristol Grammar School is a very fine school. It was founded in 1532, when Bristol was pretty almost the major port in England. It was set up to educate the children of merchants at the time, and had a long distinguished history.

Now the time I went there in the 1930's it was mostly a private school. About 75% of the students would have been fee paying, mostly from the merchant classes in Bristol. But the school had a grant from the London Government, on condition that they provided a limited number; about 40 places a year, to the best students in the state system, in the local schools in Bristol.

So this was a very competitive system to bring in these other children. This is called a direct grant school because the direct grant came from the central government. It was a school where the standards were high, but they were made much higher I think by the competition brought in by these students from the local schools. The students in the local state schools, of course, competed very hard to get into Bristol Grammar.

It was the best thing you could do. You couldn't pay fees in the city. So we got a number of very talented students on that basis. It was a highly competitive situation, and a great contrast to the school that I had been to in Burnham.

DSM: When you entered Bristol, did you feel that you were well prepared, or was this a terrifying experience at the age of 10?

JP: Well, I think I was reasonably prepared. I was probably already interested in mathematics at the time and I was fluent in the numbers, that sort of thing. So I didn't have difficulties merging in myself.

DSM: This was your first time away from home?

JP: This was my first time away from home at the age of 10. This was quite complicated because being 30 miles away there had to be an arrangement made for weekly boarding. I had to travel to and fro the weekends by train at an early, early age. My younger brother started doing the same thing later. I had to take him to and fro. So it was quite difficult and quite challenging.

Then of course the war came, and when the war started the boarding arrangement ended. It was no longer available and indeed it was undesirable for parents to leave their children overnight in a city like Bristol if you could avoid it. So from 1939 onwards I had to make this journey daily, 30 miles there and thirty miles back to school by train so that was quite a challenging period.

DSM: How old were you when the war broke out Dr. Pople?

JP: I would have been 13. A teenager.

DSM: What are your most vivid memories of World War II?

JP: Walking through the city of Bristol the morning after it was destroyed the night before. That's unforgettable. Bristol was a medieval city and had beautiful streets, which were built in 1400-1500's. They were very well preserved, and my parents had often taken me to show me this. They used to walk through it everyday on the way to school.

Then this one day it was no longer there. It was just a pile of timbers. It had been there 500 years and it went in one night.

DSM: Where were you when the war ended?

JP: By the time the war ended I was in Cambridge.

DSM: Were there teachers, parents, and friends before you entered the university that really made a difference in your life and career?

JP: Oh very much so. The teachers at Bristol Grammar were extraordinarily able and gave an amount of time to me personally. The history is a little complicated. I said I was interested in mathematics as a child. Indeed my mother tells me that when I was extremely small, as soon as I could learn to count, they couldn't stop me then.

I became very interested in mathematics actually at the age of 12 when I was at Bristol Grammar. I actually started a research program of my own on things like permutations. I sorted out the theory of permutations. I was astonished to find that it already existed a week or two later. I learned calculus on my own at the age of 12 by actually picking an old textbook out of the wastebasket and reading from cover to cover.

DSM: Did you do differential or integral first?

JP: You do differentiation first then integration and you go all the way down to differential equations.

DSM: At 12?

JP: At age 12, and on my own. I never told anybody about this, that I knew all these things.

DSM: Why didn't you tell?

JP: I think one is afraid of other students making fun of one if one knows too much at the time, but I was extremely fascinated by mathematics. It was not known to the teachers for 2 or 3 years, and then it sort of came out all of a sudden when it was discovered that I had already covered most of the curriculum. Then my father got called in for a special interview and so forth.

From then on it was decided that I would be coached for the Cambridge Scholarship Exam. Again, at this time it was very much a matter of competition between various high schools or these grammar schools in all the cities of Britain. Each one had one of these superior schools and they competed very strongly with each other to get their students into Oxford or Cambridge.

DSM: So you took this exam in what year?

JP: I took the Cambridge Scholarship Exam twice; in 1942 and 1943 by the time I was about to graduate from high school. When they decided to put you in for an exam like that you were given an extraordinary amount of personal attention. So for the last 2 years that I was in Bristol Grammar, which had been 41 to 43, I received many, many hours one-on-one coaching from the senior mathematics master and the senior physics master in the school. These were the 2 top positions in the city in teaching the subjects. So those 2 individuals were extraordinarily helpful to me.

DSM: Now in 100, 200 or 300 years when this interview is looked back on the methods of pedagogy are going to be of interest. How did they exercise you when they were tutoring you? Did they assign problems?

JP: Well they assigned problems to me individually and I would produce solutions and they would then go over them with me. Sometimes we had some to and fro. I would suggest better ways of doing things and they would show me and so forth. So it was a beginning in ready and research.

DSM: Why did you not stay in mathematics with this wonderful beginning?

JP: Well I did for a long time. I was, as I say, a mathematician and my main interest was in mathematics. Then during the last 2 years of high school in Britain the practice was to specialize. You finish your general education at 15,16 and then you specialized in subjects of your choice. I specialized in mathematics and physics. So the mathematics teacher and the physics teachers coached me personally for about 2 years. This is very different from the American system where the general education goes on until you leave high school.

In Britain you're expected to finish that by 15 and many people left school at that stage. After that you took the so-called "higher certificate," and under certain circumstances such as mine you attempted to get into a university by scholarship exam. So this was the way in which people like myself and others who had come in through the state schools managed to move their way up into the best universities.

JP: As you grew in a very special time and place in the history of the world as a child or as a young man who were your heroes? Who did you particularly admire?

DSM: Well that's a difficult question to answer, I think. Probably the answer is the people who were heroes were mostly dead. They're among scientists and mathematicians. One admired people whose work was complete and sort of branded and well established, beautiful and so forth. If you asked me about the people who were sort of a generation before mine, were they heroes to me or not? The answer is probably not because I think young people tend to be rather irreverent. I seem to remember people some 20 or 30 years older than me, and one tends to remember them for some of their flaws rather than their accomplishment. One changes that view in later years. I find it hard to say honestly that I thought the people who were 20 years older than me were heroes to me at the time. Undoubtedly, I learned much from them. I also used their influence in later work.

DSM: Did you ever think that you would perhaps be considered a hero?

JP: No, I don't think so. I think I was nervous to some extent about what would happen to me. I was conscious that a lot was expected of me by my parents in the first place. They always told me, "We want you to do something big." And of course all this attention that I received, which was a very large amount considering the large number of other students in the school, I felt that a lot was expected of me. As a young man one is nervous about whether one is going to come up to expectations.

DSM: I am going to ask just 2 more questions. One is about undergraduate life at Cambridge. Can you just talk a little bit about your experience there?

JP: Well that's a very abnormal undergraduate life because it was during the war. I should explain, of course, that during the war Cambridge was almost empty. Everybody was drafted into the Army or Navy or Air Force at age 17, and very few people were permitted to become undergraduates. The actual program that existed, which I became a member, was one in which an extremely limited number of people were taken into the universities to train them rapidly, and briefly to become active in the sort of theoretical part of the war effort.

There was a scientist who was a personal friend of Churchill. Originally his name was Lindeman, a quite well know Physicist. He was an extremely important person in the history of World War II in that he personally persuaded Churchill to devote a lot of effort to bringing science into the war effort. So there was a very high level directive that a limited number of people were to be selected out of the high schools in subjects like mathematics and physics. They would take them through the degree course very quickly, and then move into things like operations research, research on fluid dynamics in connection with the harbors and Normandy invasion, code breaking, all these things, development of radar. Many of these things were carried out by a very young man who had gone through this program.

DSM: I was going to say you were very young at the time. Did you ever get into the war effort?

JP: No, you see what happened was people who were 2 years older than me, for example, Freeman Dyson at Princeton who went through exactly the same program 2 years earlier and graduated from Cambridge in 1943, he had an unbelievable career as a boy of 19 or 20. He advised the Air Force about their bombing strategy and so forth. In my case I went as an undergraduate in 1943. I was only an undergraduate for 18 months and I graduated in the spring of 1945 on the day the European War ended. So in fact, I never got into the war effort.

DSM: Well, I could continue my questions for another hour, but this will be the last one from me and then I'll turn this over to David. Let's talk about personal pleasures. What are your personal pleasures, things you do for fun?

JP: Science is the fun. I'm interested in music, drama and so forth, but I don't take any very active part in other things. My wife is a pianist, now retired.

DSM: We didn't talk much about your family. I'm going to cheat and ask one more question. Brothers, sisters, how you met your wife?

JP: I have one younger brother who followed in the same footsteps as myself school wise and actually went to Cambridge also, but after the war. He entered my father's business and the business was expanded from being one store in a small town to a chain of stores in the west of England. He had quite a successful career in the family line.

My wife is a native of Cambridge. She was my piano teacher. So I learned the piano from her while I was a graduate student. I met her in 1948 and we were married in 52.

DSM: Thank you very much. I'm going to turn this over to Dr. David Allison. It's been a real pleasure.

DA: Did you know Freeman Dyson?

JP: I've met him, but we did not overlap. He had left just as I became a freshman. We went through the identical program.

DA: Let me pick up the story at Cambridge after the war when you, as I recalled, stayed on there to teach.

JP: Perhaps we should go back a bit.

DA: Where would you like to start?

JP: I didn't really answer the question fully about my undergraduate experience in Cambridge.

DA: Let's talk a little more about your undergraduate years at Cambridge then.

JP: I was an undergraduate for only 18 months during the war. As I had indicated it was a very crowded curriculum. One had to essentially take the whole degree course in that short period. Cambridge was very empty although some of the colleges were used as brief officer training sessions. But at the end of the year, as I had indicated, the European war finished just about at the time I was taking final examinations.

Of course the bureaucracy didn't stop and I was still dragged out of Cambridge supposedly to help the war effort, which was still continuing slightly in the Far East. The government really didn't know what to do with this group of people by 1945.

So I was sent to industry to supposedly help finish the war off. I was sent to the Bristol Airplane Company, where I worked there for 2-1/2 years. But that was a period when there was very little to do so I was more or less sidelined for a couple of years. I spent most of my time writing the government department trying to get back to Cambridge, which I eventually did in 1947. I began what you would call graduate school in this country in 1947. I then took the one more year of mathematics examinations.

At that time I made the decision that I would use what mathematical talent I had to go into some branch of science, pushing it as far as I could.

DA: That's a fairly significant decision in your career. What were the factors that shaped it?

JP: Well, I had this long 2 year period when I was doing nothing and sitting around wondering what to do with life, thinking about all sorts of possibilities; some wildly impossible. It's like becoming a writer. But, I eventually decided that I'd better use what talents I had to be as effective as possible. So I decided to go into science as opposed to being a pure mathematician. I'd probably thought that I couldn't make it too far with pure mathematics.

DA: So it was a mix of thinking about what that would be like and having an effect in pursuing signs.

JP: Yes, I think so. In fact I remember on the specific day I made this decision that rather than thinking I can do anything I'd better concentrate on something I can do and possibly do effectively. I didn't pick on chemistry immediately. I decided that I would go into applied mathematics, mathematics applied to science.

DA: When you went back to Cambridge what was the atmosphere like for you?

JP: It was totally different because this was 1947, 48, and of course it was crowded with people, undergraduates who had come out of the Army. So, the average undergraduate was about 25,26 years old. They had children and wives and so forth as opposed to when I was an undergraduate myself and the place was empty. So it was very crowded and I had become very vigorous because the faculty who were mostly missing during the war were back. Many of them at a very vigorous stage in their careers so Cambridge in the late 40's and 50's was very hectic.

DA: I guess there was a great appreciation of the role that science had had in winning the war in Britain and the United States both.

JP: Indeed, the people who came back from the war ultimately became very famous scientists. People like Fred Hoyle, Francis Crick, all came out of war efforts and really moved into other branches of science as soon they got back to Cambridge.

DA: As you were doing this advanced work were there particular professors who shaped your own view of science and how to apply it?

JP: The first year I was back I took all the advanced courses, what would correspond to first year graduate work in this country. I was looking for a field that I might work in. I did actually attempt to work for Hoyle. He was the first person I approached. I had an interest in the theory of liquids, again, looking for a general field that I could explore.

I was feeling that solids and gases had well-established theories and liquids were going nowhere. I thought that this might be something that I could do. He actually gave the course on statistic mechanics and I approached him, but we didn't really get any meeting of minds. He was interested in astrophysics so I didn't follow that up. Then I approached John Lennard-Jones who is giving a course on molecular orbital theory. He accepted me so I went to work for him. He had been developing the theory of liquids before in the 1930's, but moved his interests into statistical mechanics at that time. After one year I essentially entered chemistry then in the summer of 1948, starting to work with Lennard-Jones.

DA: And this is when you first really got serious about quantum mechanics at an advanced level?

JP: That's right, I had taken courses. In fact I took quantum mechanics from Dirac while I was an undergraduate during the war. I don't think that I understood it very well.

DA: That's kind of from the horses' mouth, isn't it?

JP: That's right. Well, you're asking about heroes when I was young. Dirac gave this course on quantum mechanics. The students' attitude was, well I suppose Dirac was just over 40 at the time, but everybody thought he was an old man who did some great work a long time ago. He was not in it much longer.

DA: Was he much of a teacher? Do you remember him?

JP: He was too formal. He essentially read from his book. If you went and asked him a question afterwards his response would be more or less a paragraph out of the book. So I did find it a little hard to connect quantum mechanics even though it was a rather beautiful, elegant presentation on its own. I found it difficult to connect it to real problems at that time that I had learn to do in other ways.

DA: Did you still work in water pretty much right away?

JP: That was my ambition when I started graduate work, which had been in the summer of 48. So we did work on the structures of molecules first of all. The pitcher of water as having bonds which is kind of the centerpiece for hydrogen bonding in water. Then I followed that with a paper on the structure of the liquid as best one could do it at that time.

An interesting feature of that was, again talking about heroes; part of my thesis was attacking what Pauling had said about liquid water. Pauling had published those things on liquid water in which he estimated how the hydrogen bonds were broken simply by measuring the heat that you put into water to heat it up from zero degrees.

The liquid you could then find how many of the bonds were broken simply by simple division. That's really not a bad approach because what happens, of course, is that the bonds begin to bend and they're flexible. That was the main thrust of my thesis material. So, it was an attempt to explain properties of liquid water in a more realistic manner than Pauling had done before.

DA: So much of your later career revolves around the tools that you had to use. I'm curious about the tools that you had in the time you did your thesis to do your research?

JP: Well, the tools were very primitive. One needed to do some computation, but they were done primarily with a very crude calculator. I used to spend all day going forwards and backwards to subtract.

DA: So you needed calculator precision. It wasn't all slide rule computations?

JP: No, I hardly ever used a slide rule. It was always done by actually putting numbers in.

DA: There was a little work going on in computing in Britain at this time. Did you know anything about that, or did you get involved in it at all?

JP: Yes, well I did. I was aware of the computing experiments in Cambridge. That was the Edsac machine. I went to look at it and saw it demonstrated. It was at that stage adding 3 plus 3 to give 6 with some moving of cables around. I was not impressed at the time I must say. I did not realize as I should have done, that this might be something that would be very important in the future.

I did not really get into the use of computers seriously until I came to this country in 1964. I regret that now. Actually computers in Britain were quite advanced at the early stage. Alan Turing was in Cambridge at the time I was a graduate student there. I never met him, but I am very conscious now that there was a lot of missed opportunity.

DA: Well I'm not sure how much of this would have been available to a graduate student at that point, but I know there was a lot of interest in numerical methods and thinking about them, but you say the technology was primitive.

JP: Graduate students did move around a lot from one department to another. Certainly we had the opportunity to go and listen to seminars in the mathematical laboratory. There was a great deal of mixing of the departments. They were all very close together which they're not anymore. Cambridge is spread out. The Physics Department is out to the west of the town and Chemistry is to the south and they don't meet anymore.

But in those days Cambridge was very central and one used to go to Physics and Biology all within the same general area.

DA: It seems to me in some ways the work you began with your thesis has characterized a lot of your research as you've gone on. How would you talk about the fundamental problems that have interested you throughout the career? What is it that you have really focused your attention on in your own words?

JP: Can we go back a minute?

DA: Sure.

JP: While I was a graduate student, and shortly after, I had a lot of contact with the group in the Physics Department which was attempting to solve protein structures and DNA so I knew Watson, Crick, Perutz and Kendrew quite well. In fact my work on hydrogen bonding came to their attention and I did, in fact, have a period when I was in close touch with them.

They wanted to ask me what I knew about hydrogen bonding, which they were beginning to suspect was playing an important role in DNA. So I had several mock sessions with them. I don't know if they were very successful and I was not really familiar enough with the compounds involved to be of much used to them.

DA: Did you ever think that you might do work with them?

JP: Well, I probably should have. It was somewhat of a missed opportunity.

DA: You thought these guys were going nowhere with this?

JP: I thought they were possibly over ambitious. That was wrong. One used to go over to coffee in the Physics Department, Francis Crick would hold forth everyday on how he was going to solve the problems of life and so forth. It was an area where the interdisciplinary things showed up quite strongly.

DA: Must have been fascinating. And, now to look back, as you say, often that doesn't happen as much now.

JP: That's right, yes. Communications between different disciplines don't happen at all easily. They don't happen in American universities to the same extent. Another aspect of Cambridge life, talking about communication, is the college system and the college dinner tie table where you mix different faculties within one college every night.

So you tend to meet historians and lawyers and researchers and they have a great deal of interdisciplinary conversation. Although attempts have been made to do that sort of thing in some American universities they've really never caught on I think. Though at Cambridge it was a great.

DA: It's interesting that you had the 2 experiences there. The during the war experience and then followed by the post war boom, essentially in education.

JP: After I got my Doctors Degree in 1951 I became a fellow and then I became a staff member and taught mathematics. I was on the mathematics faculty for a number of years.

DA: So even though you had thought about applying yourself in Science you stayed in the mathematics faculty?

JP: That's correct but there's a long tradition for this. It goes back to Weston, Newton.

DA: I was going to say Newton himself is a good example.

JP: And even until quite late the only subjects you could graduate in in Cambridge were mathematics and theology. You went into other subjects after that. So many, many people on the mathematics faculty were in theoretical physics or fluid dynamics, that sort of thing.

DA: So your research was continuing along the lines you started your dissertation?

JP: My initial chemistry research was when I was teaching mathematics.

DA: We were talking a minute ago about how you would formulate the critical problems that you started looking into at that time.

JP: I think the key feature of my work I formulated shortly after my degree. My degree was on liquid water, but then I decided to turn my attention to chemistry as widely as possible. That leads one to the problem of how you're going to make progress with the approximate solution of quantum mechanical equations. There's a very famous remark by Dirac shortly after quantum mechanics was developed, in the effect that the fundamental laws of the whole of chemistry and most of physics are completely known. The only trouble is that the equations cannot be solved.

That was true then. It's still true now. So the key question comes up that to make progress you have to necessarily make some approximations, but how are you going to proceed in a systematic way? The concept which I formulated and decided on was essentially what I call the theoretical model chemistry concept. That is the idea that given you have to solve equations approximately, have a well defined set of approximations such that they can be lead to well defined answers, which will not be correct answers but they'll be approximately correct, then you can apply the same set of approximations essentially to all chemical processes. So given one set of approximations you have an entire model chemistry.

If that model chemistry is good enough, it will ultimately have predictive value. This is as opposed to the other concept which some people follow, in which you take each problem separately and you do the best you can; you do the best approximation for this molecule, best approximation for this molecule. My concept was that one set of approximations could be applied to the whole of chemistry. I formulated this general plan around 1950. Even though computers were not available I could not carry this out, but it was kind of a challenge to work towards in the future. The initial things I did along these lines were very approximate, but none the less of this kind of well defined, widely applicable.

It's that general concept of the model chemistry which is, something which ultimately fitted in very well with the development of computers and, of course, follows what people do in many other fields like meteorology and so forth where you take models and apply them on a large scale to a large amount of data.

So in more recent years it's been possible to develop models which can be applied systematically. Today we do this by essentially taking a model and testing it against almost all known chemical facts. If you talk about the energy of a molecule, how stable is it, and you look through the experimental literature and how many molecules have their energies completely determined by experiment, the answer is a few hundred. It is now possible to take your theoretical models, apply them to these 300 cases and to actually get some statistics on whether the theory is successful or not. If the theory is successful and you can measure how successful; then of course, the model has predicted value and you can begin to use it to predict properties of molecules which are not yet known or maybe controversial, speculative. That's the way the theory is developed.

DA: In the early days when you were a young professor pushing this notion how was it accepted by your colleagues? Or was it?

JP: It was largely not accepted in the early days by practicing chemists. I think there was worldwide resistance but it was strong in Britain. I recall immediately after I got my fellowship at Trinity College, which was just after my doctoral thesis, at the dinner celebrating this, I sat next to the distinguished organic chemist who's a fellow of the college. I was described as having been awarded the fellowship for my work in theoretical chemistry; this is my thesis on water. He said, "Well I don't think you should call yourself a chemist. You should not call yourself a chemist until you've discovered something about chemistry that chemists don't already know." He didn't think I had qualified at that stage. But those I think, now have changed.

DA: Yes. You mentioned that your modeling required, even for the early days, significant calculation. How did you first get involved with computers? Did you do that at all in Britain before you came over? You said most of your work came after you came to the United States, but I wondered if you began to even look at kind of thing?

JP: I began to look at it. Again, I was slow in taking it up. In the 50's I continued to use electric machines where you pushed buttons. I actually did inquire once or twice about what possibilities there could be in using computers. I got sort of negative responses. For example, solving matrices, which is an important thing in applied quantum mechanics.

I think as late as the mid 50's that was described to me as being a long way off, "We won't be able to do that for a long time." So I used to do these things on electric calculators. I should have been more persistent I think, because they did begin to move ahead very rapidly.

Then there was a period in my career when, because after I had been in mathematics for a number of years, I became disillusioned about teaching mathematics. I really want to do science and I was spending too much of my time on mathematics lecturing. So I moved to an appointment at the National Physical Laboratory, which corresponds to the Bureau of Standards in this country. I was there as an administrator for a number of years. At that time I began to think more about using computers. Didn't really get down to it until I moved to the U.S.

DA: So when you left Cambridge it was as much wanting to focus more fully in science.

JP: That's right. That's exactly right, yes.

DA: Did you have that opportunity when you went to the National Physical Laboratory or did you end up doing a lot of paperwork?

JP: Yes I ended up doing a lot of paperwork. I took that view and I went there that the time I'd previously spent on teaching I would give out to administration and I would still have as much time to do research as I had before. Time wise that was probably true, but what I found was that for administration in the government department to be effective, you had really to put it at the front of your attention.

When I woke up in the middle of the night I would think about how I was going to get a new appointment in something rather than a scientific problem. So I did find that it caused my research output to decline. During that period I was not very effective, which is a major reason why I decided to leave.

DA: As we talking last night your move from Britain to the United States became something of a cause celebre. What were the circumstances that led you to come to America?

JP: I actually came on sabbatical in 1961, 62 to Pittsburgh to Carnegie Tech as it was at that time. It was immediately after that that I decided to give up the administrative job that I had and look for a position which would enable me to do essentially full time research, where a research group is my major function. Opportunities did exist in Britain but I felt at the time that the U.S. was more receptive to the development of common theory and these models that I was hoping to describe.

By that time I had been to this country many time and had given many lectures and seminars. I was always impressed, particularly with the younger students the large audiences that would turn up to hear me speak, which did not occur in Britain at the time. It was an encouraging and receptive audience. I was also offered very good facilities, freedom from any duties really other than what I wanted to do at Carnegie Tech. It was ultimately very successful move.

DA: I take it that there were some in Britain that were disconcerted by your moving to the United States at this time?

JP: Well, that's true. Moves were made to persuade me to stay but it was hard to believe that it was in the immediate interests of my scientific work to stay there. Also having been in Pittsburgh on sabbatical we had connections there and that made it a little easier for my family to move. We did have mixed feelings about it, very mixed feelings, still do, but scientifically it's been very effective.

DA: How would you compare the scientific climate for your kind of work at that time? You talked a little bit about that in terms of reception to your speaking. But in terms of resources, research interests, did you feel that work in theoretical chemistry in the United States was now surpassing what you found in Britain or were they equal? How did you look at it?

JP: Resources, one didn't worry too much about until I decided that this concept had to be married to computers sort of right from the beginning. Then that did become important. I found that Carnegie Tech, which became Carnegie Mellon shortly after I got there, was excellent from that point of view. It's a very live school in the computer field. They provided excellent facilities; free computer time when that was by no means a universal thing. In fact many other universities had their quantum chemistry program severely cut back because computer centers insisted on a sort of dollar for dollar. You've got to raise every penny you want to spend on your computer. That was not true at Carnegie Mellon. That did become a very important feature. It would have been extremely difficult at that time in Britain to get the kinds of opportunities that I had in Pittsburgh.

DA: So, was the move to computer computation something that you did on your own initiative or was that part of the deal when you went to Carnegie Mellon? Were other people as interested in that aspect as you were?

JP: Oh yes. In fact I was if anything, late in coming to that. Other people had used computers in Chicago. One school had done some computations on small molecules using computers at that time. I was by no means the first. I was in fact quite late.

DA: I'm just curious. Do you remember what kind of machines you were operating on at Carnegie when you first got there?

JP: Yes, the first machine they had there was a Bendix. They were making washing machines as though they make computers in those days, which was a sluggish machine. Their principle limitation there was that languages hadn't settled down. You'd write a program and then come back after the weekend and the language had changed. It was hard to keep up with.

DA: Were you talking in Fortran?

JP: No, we actually started in ALGOL.

DA: Oh, did you?

JP: This kept changing. After 2 or 3 years we decided to change everything to Fortran. After I had been there about 2 years Carnegie Mellon was formed with the merger of Carnegie Tech and Mellon Institute. Then Mellon Institute provided a control data machine primarily for the use of theoreticians. At that point I had very close access to a machine and became deeply involved in programming.

DA: Let's talk a little bit about how your Gaussian program and theory developed. I guess it was really during this time that it seemed to take shape, that was my sense.

JP: My research in quantum chemistry after I moved to the U.S. was initially what was called semi-empirical methods which was making multiple approximations so you could immediately apply things to large systems. Then I turned from that to essentially taking a certain approximation and then doing the calculation properly and calculating all the integrals and so forth and not leaving anything out.

That began about 1967. There were already programs available at that time of this general kind. So our program started from that and we began essentially stripping them down and rebuilding them in a form which would be much more efficient, and therefore available for computations on much larger systems than had been possible before that.

DA: So you really saw the crux of your work now to apply this information technology to expanding this idea to increasingly deal with larger and larger numbers of electrons?

JP: That's correct. To do that in a systematic way with a well-defined method, and compare with experimental data as you went carefully and systematically to see how the approximate theories developed. The very first theories worked very badly as one expects. Then one sees what's wrong with them and they were refined over the years. But the Gaussian program started in this way.

It was really initially a reformulation of existing programs with new features, which gave great increase in the efficiency of computation of the various integrals, and thereby made it applicable to a wide range of molecules really for the first time.

DA: Your work was actually in writing the code or coming up with the plans for it and then giving it to people who write code?

JP: Yes, a piece of the code, a central piece of the code which is the technique for evaluating the integrals using Gaussian functions which were actually developed some years before. We took that over and we succeeded in increasing the efficiency of the algorithm for that step. That's work I did myself by a factor of 200 or so which was a real breakthrough at the time. Then this program was made available about 1970. It became called Gaussian 70. It became used for the first time for studies of lots of molecules.

DA: And you say you had a research group there at Carnegie?

JP: Yes.

DA: How did that play out?

JP: Like most American universities, one gets a grant from the National Science Foundation. I supported several students and a number of post-doctoral associates. Some came with their own money. I had a group of probably 6 up to 10 at one stage, but that was about as large as you could handle. I work best with a small group, something like 4 post-doctoral students.

DA: So they were all doing graduate level work and had come from other universities and had come specifically to work with you on this problem?

JP: Yes, that's right. My most successful graduate students were people who had become interested in this subject as undergraduates. So they knew of my name and they came to Carnegie Mellon to work with me. I had some outstanding students.

DA: Was the thing that tended to pace the success of your program at this point technological capability? Was it the change in the computer? Was it more theoretical development? Was it a mix of the two?

JP: It was a mix of the two. For many years I used to have an index of how many orders of magnitude we had improved the efficiency of the program since we started in this sort of thing in 1965 or so. I haven't worked this out recently, but it used to be about 3 orders of magnitude by computers getting cheaper essentially; another 3 orders of magnitude by writing more efficient programs, which was our contribution. So both played a major role.

DA: So you must of started eagerly awaiting developments in the industry as they began to occur?

JP: Yes, rather so. It goes so fast that it's hard to keep up with them. We work first on this Control Data machine, which was 1964? Is that right? I think it was a famous machine in the 1960's. We bought it second hand. It had 32 kilowatts and the words were 6 bytes, so 119 kilobytes was the memory.

DA: I remember the 64 and 6600 series.

JP: Those came later. We worked on the 6600, and then the Univac 1108 machine. Then later on in the 1970's I was very fortunate to become the first owner of a VAX computer. Number 1 was delivered to Carnegie Mellon for our use, and that was a very effective machine.

DA: You mentioned that you had a continuing series of students come to work with you. Would they then turn around and take these techniques both to other universities and into industry? Did your work tend to spread through them or was it also spreading in other ways?

JP: It spread through them. My students moved to faculty positions in other universities. They took the program with them, developed themselves further, continuing in collaboration with our group. Others have got into the commercialization of programs of this sort, which started I suppose 10 or 15 years later. There are now a total of 4 commercial companies, which are run by former students of mine.

DA: Talk a little bit about the commercial application. It's hard sometimes for people to understand the value of analyzing chemical reactions at a very fine level as you do and understanding quantum relationships. What difference does that make in the practical application of that knowledge?

JP: Well, it enables one to understand the mechanism of the reaction when a molecule comes apart or rearranges to form some new isomer. We are able to say something about the root, the way the nuclei move in such a reaction, how much energy is needed. Then you might want to modify the molecule in some way by putting on different substance into it and how that would change. Would that speed up the reaction or would that slow the reaction down? You can now quite often predict this by doing the theoretical computation on the amount of energy needed. That would then give some indication of how new materials can be produced, which might go through some reaction more effectively or less effectively.

DA: That totally allows you to do designer chemistry, as it were.

JP: Yes which of course people have always attempted to do experimentally, but we can supplement this and sometimes do it more efficiently, and sometimes find new features that they may not think of, or may find difficult to evaluate.

DA: We've talked some about the developing of computers. I guess at a certain point you began to really get into the super computer era.

JP: Yes.

DA: I'm curious as to the current state of technology and what it is allowing you to do to, and how far your theory has been able to be developed?

JP: The super computers have made a difference in the application to the largest possible systems. I think the great majority of computations, certainly the ones that I did, and now ones that most people do, can be done now on very small computers like a small Pentium, which I have at home. But the trouble with the methods, which are effective at the present time, is the cost of doing a computation goes up very rapidly with the size of the system. Actually it's the 7th power of one part of the calculation goes up as the 7th power. So if you want to examine something twice as large, you may have to spend 100 times as much in computation. So it's really in pushing existing methods to larger systems that super computers are available or useful at the present time. I don't think that they're always used that way.

It's often happened in these super computer centers that they take this big machine and they parcel it up into small pieces and hand them out in small quotas. That's the sort of work that could well be done on small machines at home.

DSM: But you are now able to do what 30 or 40 different?

JP: We have criteria on what we mean by really well which is really reproducing experimental accuracy. That can now be done for molecules easily, 30 electrons or so, and pushing it hard on a Cray machine up to 50 electrons. Now there are other models, which are less expensive, but they are not as yet as effective. They are getting close, but not as yet as effective.

DA: As the complexity that you can attack becomes greater and you can do 50, and maybe later more electrons, do you see major new areas of knowledge opening up, or is it just sort of an evolution from where you are today?

JP: I think within chemistry that's true. One is never supposed to say that nothing new is going to come, particularly when you get older. I think that's been true for the last 20 years or so. There have been steady improvements. We've been able to do bigger systems with better precision partly because of improved algorithms partly because of the rapid improvement in the computer hardware available.

DA: I tend to think of organic chemistry somehow becoming more and more open to this type of analysis as opposed to the simpler compounds.

JP: That is true. We say 50 electrons. Now many compounds in organic chemistry or biochemistry of course would be somewhat bigger than this, 100 electrons almost they would be. That opens up a vast new area.

DA: Many people stand in fascination to watch designer chemistry, designer drugs and new molecules being fabricated almost at will with chosen properties. That worries a lot of people to think that man has that kind of power over nature. Does it ever worry you? What do you say to people who wonder how much power we actually begin to have over the world around us?

JP: It worries one, but it's enviable. It's part of the human condition that science is going to proceed. Trying to hold it back for any reason is not going to be effective. We do and should worry about what people do with science, but science produces opportunities for mankind. It's dangerous as well. We have to live with that. I don't find proposals to limit research to be really viable or sensible.

DA: If there were one area of new knowledge that you could see opening in the next few years what is your greatest dream in terms of how your theory will get applied?

JP: Clearly they're talking about new areas of science generally. The biological area has been a rapidly expanding one. I think one understands more and more the nature of living material as it exists at present. I suspect there's a very big future area in science and chemistry whereby one will have some form of self-reproducing molecular system which begins to approach life, possibly based on an entirely different set of underlying reactions.

Life as it's explored now, biology involves very specialized compounds, and it's hard to believe that that's the only way that life could exist. I would think that ultimately it's going to be something that will spread into any new areas.

DA: So the whole notion of self-reproducing systems may be made on a different structure than what our friends Watson and Crick came up with?

JP: That's absolutely right. One would imagine that had life started on some remote planet elsewhere in the universe that it would probably be totally different. It can still be a self-reproducing system which would develop in a somewhat different manner.

DA: You talked earlier about the special conditions under which you got your start in education. I know that throughout your career you spent quite a bit of your time working with the people who work with you; that is developing strong research groups, working with students, and many of your students think very highly of you and the effects you had on their career. How important has teaching and mentoring been in your career in science?

JP: Oh I think it's absolutely vital. The great joys in being in a field like this is to be able to interact with students very much in a to and fro basis to exchange ideas and to help them develop their own concepts and put them forward into viable form.

DA: What is the secret of how you work with them? What's your style?

JP: I tell them rather simple things, to think about things fundamentally, go to the core of the problem. I tell them to think about it before reading literature too fully. I think that's an important thing. I think too much of a tendency in this country for education is for people to say that you have to read everything up to date before you start doing research.

I think it's desirable to identify your problem, to think about it, see what you can formulate yourself and then when you've made some progress with it, then go to the literature and see what other people have said. You may well find that you've done something different from what they've done. Going back to the beginning of this interview, this is a concept which goes back into my childhood. This is going back to when I was 12 years old. When I first started doing science I was fascinated by the idea that if one started science all over again, or one started science in a community which was disconnected from the current civilization, would the same concepts come out? Would we look at the universe in terms of atoms and electrons and so forth? Would it be completely different? As a 12-year-old child, one does odd things. I actually decided that I would attempt to do this myself and not listen to the teacher and see if I could formulate things myself. It didn't last very long of course. I didn't get very far. I did have this concept that you should think independently before reading everything that is already know. You may come up with something fresh.

Then I also tell students to go step by step. Always start with the simplest thing. Only introduce complexity if it is necessary. Don't introduce complexity just to show off how clever you are, which some people tend to do. So there are a few simple precepts, which I think one should follow in research.

DA: Dr. Pople, thank you so much for your time and granting us this interview for the archives.

JP: My pleasure.