James M. Stewart received the 2001 Fankuchen Award for his suite of crystallographic computer programs, XRAY63, later known as XTAL. As part of the ACA History Project, he recounts here the influences that shaped his scientific career. Jim's full narrative will be deposited at the Center for the History of Physics (AIP). This is the first of a series of narratives by individual crystallographers. If you would like to contribute your story, contact Virginia Pett, pett@wooster.edu.

I had the mixed good fortune to be born in Port Angeles, Washington in February 1931 at the time when the Great Depression was firmly established in the land. My father Charles R. Stewart was born in Selkirk Scotland, my mother Mary E. Stewart nee McDonald was born on the upper peninsula of Michigan. I like to say it was a marriage concocted in hell. A committed Women's Christian Temperance Union devotee and a dram-fancying Scot!

Jimmy Stewart and Uncle Charlie, 1934.

My family constituted my introduction to science. My father was a literate and a charming Scot who could quote Burns, some of the romantic poets, and sing in addition to his skill as a plumber and being dedicated to stamp collection and the geographic knowledge that instilled. He was, in the tradition of his father, a fisherman. I got very early opportunities to see lead melted and used, pipes threaded with the difference between tapering pipe threads and cylindrical machine threads explained. When my parents got to Port Angeles they set up a plumbing business there which proved unsuccessful. My mother, as she put it "kept the wolf from the door" by working in a local grocery store. Although she had only six years of schooling, she was a quick study and took in the details of the trade. My Uncle Charles W. Alward was an engineer on the Port Angeles and Western logging railroad. So that meant at a very early age I got to see and be held in the cab of the Shay locomotive that he drove. And as the years went by I got information from him on all sorts of aspects of the logging operations and the operations connected to the Alward farm. Some of the lessons were frivolous such as the day I found out about an electric effect. Walking with Uncle Charlie from the house to the barn he held out his hand and said: "Take my hand Jimmy." Which I did only to find out that he, in his rubber boots, had his hand on the electric fence. Hello! Pay attention!

I was carrying kindling from the woodshed very soon after I could walk and delivering groceries for Stewart's grocery store from the time I was in grade school. My family all treated me as being able to understand and do. They must have thought that I had talent, but like Uncle Charlie and the electric fence lesson, they were careful to be sure I didn't get any ideas of myself that are like the ones being touted in the 21st century about building self image. One particularly valuable role was being the one to run and clean the cream separator on the Alward farm. Aunt Margaret milked two Guernsey cows. In those days the valuable product was the butter fat. The separator is a type of centrifuge that can divide the skim milk from the cream. The cream could be sold to the local dairy and the skim milk can be added to otherwise waste foodstuffs into slops for the farm's pigs. The device consists of a crank for motive power, an upper chamber for the raw milk, a stack of pleated disks on a central shaft and two chambers with spigots, one for the less dense cream, the other for the more dense skim milk. Assembling it, using it, being its power source, and finally cleaning it was training not commonly available to the majority of my classmates.

At Bellingham High School we got to do many interesting laboratories that have now become inaccessible to beginning chemistry students. For example — we synthesized rayon, nylon, we built a mercury barometer, and we generated oxygen from mercury oxide by heating it in a test tube with a Bunsen burner. After Western Washington College of Education, the next significant step in life was getting married to Bernice Dorren and starting graduate school at The University of Washington.

Jim and Mrs. Lingafelter at ACA meeting, 1980s.

At UW Professor Lingafelter, an X-ray crystallographer, was an outstanding mentor and a teacher with great knowledge and talent. There were also great moments in the ethics of science. I was in the process of checking out a bond lengths and angles program for the IBM-650 when there appeared a paper by Lippert & Truter on the crystal structure of monoaquobisacetylacetonatozinc where the authors published their bond lengths

and angles. Since Henry Mongomery in our group was scooped by this publication I tried to compare their results against mine. There was something clearly wrong so I consulted Lingafelter. In an instant he saw what I didn't: that the authors had used the monoclinic cell angle β* for β. Setting that right made the two results agree within the precision of the two data sets. At that point Lingafelter wrote to the authors and pointed out what he had discovered and suggested that they might cooperate in posting a correction in mutual interest. Montgomery & Lingafelter published their structure, giving credit to Lippert & Truter. In a subsequent paper Truter & Lippert expressed their gratitude for the error notification.

The first computers that I got to work with were located in the administration building. The research people got to use them on second and third shift. They were early IBM accounting machines. Professor Lyle Jensen had mastered their use for doing Fourier analysis of crystallographic data and I got a chance to be a "helper." But before too long the research people got their own computer, an IBM 650.

It was on the IBM 650 that I got my first taste of computer programming. In my life it was the most amazing intellectual pleasure I'd ever had or have had. It involved bringing to bear all the step-by-step details required to process raw data into useful results. Moreover, the 650 brought its own complications to problems. The storage was minimal, just two thousand 10-decimal "words" or 20 kBytes. That space had to hold the program and any data needed in the calculation. The memory medium was a rotating drum. In order to fetch words from the drum quickly, the programmer had to take into account that if instructions were not issued in a timely way, the registers in which the calculations were carried out would be delayed until the next required word rotated to the "read or write head." So you had to be sure to store your variables at locations separated by the optimum number of words if you wanted maximum speed. Now all of this is useless information. I just give it here to give a flavor of where many hours of my life went. You may think wasted, but I'd argue that it was fun, it made my reputation, and it put shoes on the baby, as one of my mother's aphorisms would put it. The next step up was to the IBM 709, the first really big machine the university got in. This was the machine on which the XRAY system was developed.

After accepting a two-year appointment with Professor P. M. Harris at The Ohio State University I was put to the task of getting the IBM 650 programs up and running that I had brought from UW. I also got to work on refining the structure of the explosive RDX (1,3,5-trinitroperhydro-1,3,5-triazine). The structure had been solved by direct methods, but not yet refined. Doing crystal structures in 1958 was a several-year and sometimes several-student process. It was on the IBM 704 at OSU that STARTX, the first program of XRAY was coded.

Returning to Seattle, I was given teaching duties because of an illness that kept Ed Lingafelter out of school for a year. The only course I remember doing during that time was an elementary one in physical chemistry for medical technicians. But the best part was getting back into the very active cooperative programming scene. A graduate student from the Protein Crystallography group, Darrell High, and I hit it off very well and continued generating a "system" of programs for the solution, refinement, and reporting of crystal structures called XRAY63, a plan that would turn into my major contribution in the field.

It was not till years later that Syd Hall and I decided to create the XTAL version to enhance transportability among computers. At one of the IUCR summer schools I met Syd Hall. Each of us had been working on writing code to produce all the triplets for doing direct methods. My post-doctoral student, Roger Chastain, had generated an excellent code that was very fast, Syd had generated a code that was equally fast but used an entirely different algorithm. On comparing how it was done in each case we realized that the methods were quite different, but could be used in combination. Thus began a long collaboration that lasted till I faded away at the University of Maryland College Park, and Syd took up the care and feeding of XTAL from his base at The University of Western Australia in Perth.

Jim in Scottish dress in front of his "memorabilia wall" that includes the plaque for the 2001 Fankuchen Award, 2010.

Because of people's interest in XRAY and XTAL I was privileged to travel the world and learn more about what was needed to do crystallographic computations. However, without a doubt, for me, it was the interactions with the people who built and used the system that I treasure most. It was through their effort that XRAY came together.

We still have judgement here, that we teach but bloody instructions, which, being taught, return to plague the inventor.

–MacBeth Act I, Scene VII

Those of us who used XRAY/XTAL remember the error messages, generated randomly from a file of quotations ranging from "Ozymandias" by Shelley to Charlie Brown.