

Memories of Jim Stewart (1931-2010)



Our colleague, Jim Stewart, was a renaissance man. He was a devoted, energetic, and patient educator who had an uncanny ability to detail, systemize, catalog, and recall which allowed him to immediately quote from history, literature, and recent newspaper/magazine articles. New topics under discussion or questionable points prompted his immediate quest for answers which were quickly returned. Jim touched many of us with his wit and thoughtful comments. An avid

environmentalist, he practiced its principles long before that term gained its present popularity. His Great Depression upbringing together with a deep understanding of thermodynamics were evident in the homes he designed and built, in his choice of automobiles, and many other aspects of his life.

We met in 1956 at the U. of Washington as graduate students under Ed Lingafelter. Jim's long involvement in crystallographic computing began there on an IBM 650 computer. Jim's subsequent consulting at Sandia National Labs on programming, mutual visits over the years, and personal interactions of our families provided the intertwined thread for our long friendship.

His quest for a solar-heated, energy efficient house began with the "Hyattsville" one, adjacent to the University of Maryland (UMD), continued after his retirement with sequentially; the "McConnellsburg Cabin", "Torrie" (a 4 story house taking advantage of the picturesque Pennsylvania ridges), and finally the one level in-town house, "Ayr But An Ben", which also had a walk-in basement. Slightly different, but potentially improving energy efficiencies were used in all of these *via* insulation options including solar window input and leaning sarcophagus-type hot water heating, foam insulated roof/wall panel construction, total exhaust air heat exchange systems, ground source heat pumps for hot water and house heating and use of insulated concrete panels for basement sections. Over those nearly 50 years, meticulously kept records were maintained for various energy consumption units (purchased as # of kWh, cu ft of gas, and gals of propane @ \$\$ on dates @ mean temperature, but also each converted to GJ & totaled; a strict one on CGS units) allowing a comparison of improvements he designed into them (achieving a remarkable 3.5 times improvement in total E/floor area from "Hyattsville" to "Ayr But An Ben"). And of course, he was interested in comparing these results with my various homes because of the very different climate here in Albuquerque.

Because Bernice and Jim were avid readers, each of the houses contained enough books to fill more than 3 walls, 9' high. He introduced me to the Great Courses series of DVD lectures and would not hesitate to review the detailed thermodynamics of heat pumps to me, possibly because he was disappointed that I did not use ground source heating in my latest house.

He was keen on hybrid and future total electric cars; their drive trains and/or related motors. Again he kept detailed spreadsheets on his cars. For example, the spreadsheet on the 2005 Prius JTDKB20U653041174 had columns for gal bought, cost, MPG, T in F, true MPG, dash total gal, true cum MPG, dash gal, dash total gal, dash cum MPG, % error, % fill error and \$/gal!

We had long discussions on fair taxation and "consumption" taxes, present tax sources and their distribution; on national debt, deficit budgets, the monetary system, and gold; on free will, the origin and evolution of Christian faith, religious fundamentalism, in Islam as well as the West, and their interface with other religions. And when he judged me lacking, a week or so later the UPS would deliver a book for me to read.

I miss the weekly, sometimes more, phone conversations which supplemented the many e-mails exchanging various articles and data. I am sure that all of you who knew him will also greatly miss him.

Bruno Morosin

I first heard the name of James McDonald Stewart when I was a graduate student at Louisiana State in the early seventies. When I first joined the group my advisor Steve Watkins told me that Jim was one of his great 'heroes' in the field of crystallography. In those days, the software system that we used for data collection, reduction and structure solution was Jim's XRAY69. The XRAY package was extremely effective and educational. Whenever our group had unresolved problems we would either call or write Jim about them. He always explained the software and the crystallographic principles involved in detail. We benefited a great deal from Jim, not only because of his pioneering software system, but also because of his willingness to teach computational crystallography any time and any place.

After joining the National Bureau of Standards (NBS, now NIST) in 1983, I had the opportunity to meet Jim a number of times at the local crystallographic colloquium in Washington DC, where he was very active and gave frequent lectures. From 1986 to 1988, I worked as a NIST guest scientist, and also as a research chemist at the chemistry department of UMD under Jim's guidance. We received a three-year grant from ICDD to prepare x-ray powder standard patterns of electronic materials for the ICDD Powder Diffraction File (PDF). Jim was involved in an advisory capacity on the software for powder data collection and data reduction. I enjoyed our friendship very much. He was a great mentor, a wonderful, gentle, and humble scientist.

In the mid eighties, one of Jim's graduate students, Yuming Zhang, also worked at NIST on a project concerning the crystallite size/strain of materials. This project was co-directed by Camden Hubbard, and Bruno Morosin. The computer software suites 'XRAYL and CRYsiz', and the certification of an instrumental profile standard (LaB₆) were developed as a result of this project. Jim often came to NIST to hold discussions and to supervise Zhang. I also benefited by learning about various aspects of both the software and the principles of residual strain analysis. Zhang told me on many occasions that Jim was the nicest and most dedicated professor he had ever known.

Although Jim retired formally from UMD, his eagerness to teach never ceased and he stayed active by teaching at Juniata College for many years after his retirement. Jim continued to instill in the minds of young students an appreciation for the importance and elegance of chemical and crystallographic principles.

Jim was a great teacher and a giant in the field of crystallography. He opened the door of computational crystallography by creating the computer suite 'XRAY'. His vision and his software have transformed the field of crystallography forever. Many software systems being used nowadays are based on his concepts and the strategies applied in 'XRAY'. Jim's patience, unique way of teaching, rapport with students, and in-depth knowledge of both crystallography and computer science earned him tremendous respect from his students. I have the utmost respect for Jim; and like my graduate advisor, I will also always consider him as a great hero and teacher in the field of crystallography. His receipt of the ACA Fankuchen award in 2001 was a well-deserved acknowledgement of his great contributions. Most importantly, his influence will live on in the continued development and application of the computational areas he helped create.

Winnie Wong-Ng

My memories of Jim Stewart span 45 years; all are wonderful. We first met in the mid sixties when I was an NRC post-doc in Ottawa. Jim was a computing guru at UMD where he coordinated the development of the *XRAY System of Crystallographic Programs for any Computer*; a radical approach then as most software was written for a target machine. This was an era when computers were mainframes supported by large budgets and staff. Crystallographers faced serious portability problems with time and money being wasted on adapting programs to the different hardware types, operating systems and Fortran versions!

Jim was always a relatively shy person, except when it came to discussing computing. He then literally glowed with enthusiasm and could talk authoritatively about all aspects of the field. Jim attracted many converts to his XRAY philosophy of restricting machine-specific aspects of languages; in particular, to use only US-Standard ('pidgin') Fortran. Software contributors to XRAY, and later those to XTAL, usually became his close friends and remained so for life. I collaborated with Jim from 1968 and visited his lab and home a number of times. These were memorable and productive occasions. Jim had two main priorities in life; his family, followed closely by his computing interests. During these visits we would often work at night when access to UMD computers was faster and cheaper. Jim always dealt with family matters first, and then we'd go to do battle with the latest coding problem.

Jim was a born teacher and had the best people skills of anyone I knew. He was famous for his 'community' coding sessions when he brought programmers together to write code in real-time! This required special people skills, and Jim did it regularly. In more recent times, I believe Jim could easily have been a billionaire developer with *Microsoft* - which, coincidentally, has its HQ close to where he was born. Most programmers I know work best solo. But not Jim, he relished the interaction of ideas and egos and made it productive. It was also fun because Jim was just as apt to jump up and recite a poem of Robbie Burns or sing

a little ditty – his way of keeping the ideas and code flowing.

Jim loved anything technological, and especially autos and energy-efficient houses. The mention of autos or solar houses would always provide a welcome diversion from the intensity of coding. A fair slice of our time together in Washington, Ottawa and Perth, was spent discussing these. When I eventually installed a full photovoltaic system at home - a trivial addition compared to his efforts – he was delighted.

It was hard to resist Jim's enthusiasm for computing; it embraced relative strangers. A computing center director at UWA who gave crystallographers continual grief over access and charges, suddenly became quite generous after a meeting with Jim. He held similar sway over the UMD computing center where he was an Honorary Fellow. He routinely ran his jobs from the main control screen in the central machine room. Such access was unheard of in the days when computer managers were high priests and users were considered, well, unclean! Everyone who knew Jim has stories to tell of his persuasive powers – he had a way with people; the UN could have done with his skills.

Outside of the family, Jim wasn't much interested in social gatherings. His favourite beverage was Pepsi, and for him coffee was a definite walk on the wild side! Raised as a strict Protestant, his upbringing cultivated a lifelong interest in efficiency, reuse and avoidance of waste. He recycled drink cans before it became fashionable; he kept a fuel/mileage log on his autos and knew their efficiency to two decimal places. This frugality, conservativeness (in the truest sense of the word) coupled with a real generosity of spirit, were lifestyle benchmarks for younger colleagues – though, alas, few of us could live up to them. Jim had no apparent interest in sport. Yet he was a avid walker and would walk to work in Washington's tropical heat or polar cold rather than drive and in so doing leave younger and fitter people in his wake.

Jim's collegial approach to software development involved experts in the field directly. When the distribution of XRAY tapes became too complicated, Jim and Bob Munn coalesced RatFor and Macros into an approach that could be targeted at specific machines. A new package, XTAL, based on RatMac, was released in 1984. This remained well-supported, with 30 contributing authors, up until the late nineties when version 3.6 was placed in SourceForge as shareware. The XTAL development model depended on healthy computing budgets and widespread programming skills; alas, both have greatly diminished.

Jim's contributions to crystallographic software and teaching over 50 years were recognized with the ACA Fankuchen Award in 2001. Friends and colleagues who were fortunate enough to be in LA on that occasion were as proud and emotional as he was!

I close with a quote from XTAL. This is one of the 65 messages issued if an input error occurred - important therapy in an era when the next possible turnaround may be 24 hours away.

Fireworks ended - and spectators gone away...

And how vast and dark! - the Haiku poet, Masaoka Shiki.

No more turnarounds in this session, old friend - we'll miss you a lot.

Syd Hall