12 April 2007

To: File
From: Bill
Re: Amended Remarks for Gelato Award to Clemens

Good morning. It's my privilege this morning to speak to you about a history of significant contributions to scientific computing culminating in important contributions to the Itanium architecture and Itanium software.

The full story begins in the Netherlands in the year 1918, but I'll pick it up in the fall of 1959. I began graduate school that fall at the University of Chicago, and it was my good fortune to elect a mathematical physics course taught by Professor Clemens Roothaan.

After the first exam of the course, the grader took exception to my transformation matrices on the left rather than on the right. I visited Clemens's office to plead my case, and, after a short chat, he asked me if I was interested in computers. I knew absolutely nothing about computers, but replied in the affirmative. Clemens's next question was to ask if I wanted a programming job. If I remember correctly my response was along the lines of "Are you serious?" I didn't realize at the time that Clemens's influence was steering me to a new career path. And I remain grateful to him to this day for that influence.

Clemens was born in 1918 in the Netherlands. He began the study of electrical engineering at Delft in 1935. During World War II he was imprisoned as a prisoner of war due to a brother's activities with the Dutch underground. At the time, because of conscription by the German occupation, the Phillips Corporation was experiencing a shortage of scientific and engineering manpower. Phillips persuaded the Germans to permit them to use the services of imprisoned professors and students. This enabled Clemens to continue his scientific work, and he once told me that he believes this probably saved his life. He later was detained for a year in a concentration camp.

After the war Clemens's work for Phillips was recognized, he was awarded a Master's degree. In 1946 Clemens obtained a postgraduate fellowship in the University of Chicago's physics department. At that time the physics faculty luminaries included Enrico Fermi, Edward Teller, Maria Goeppert-Mayer, and Robert Mulliken. Maria Goeppert-Mayer subsequently helped Clemens get a post with Karl Herzfeld at the Catholic University at Washington while he continued working on his PhD thesis with Robert Mulliken. Clemens was invited to join this physics faculty in 1950, became a full professor in 1959, and remained at the University of Chicago as a distinguished professor until his mandatory retirement in 1988.

Clemens's PhD thesis established him as the father of computational chemistry. It was published in the April 1951 issue of the Reviews of Modern Physics. Until 1954 it was the Review's most frequently cited paper. It remains today one of the most frequently cited papers ever published in the Reviews of Modern Physics. In a December 2001 interview with Chemistry and Engineering News, Clemens explained that his basic idea was to use the then known construct of linear combination of atomic orbitals (LCAOs), but to treat the coefficients of the linear combinations formally rather than semi-empirically. This led to very large variational problems in which the coefficients can be determined from first principles by finding for each problem the combination of coefficients that produces the minimum energy. The result was christened the "LCAO self-consistent field theory."

It is hard to overestimate the importance of this work. Professor Peter Lykos, a longtime colleague of Clemens at the Illinois Institute of Technology, calls Clemens's work "monumental" and points out in the same Chemistry and Engineering News article that Clemens "transformed the doing of chemistry" and "marked the beginning of the age of electronic digital computers." For Clemens's methods, the use of a computer was no longer optional. Peter went on to state that "it's likely true that thousands of times each day – all over the world – chemists, physicists, and biologists use Clemens's computational methods in their work." The Wikipedia article on the history of chemistry reads "a milestone article in quantum chemistry is the seminal paper of C J Roothaan on Roothaan equations." The Wikipedia article on Clemens himself calls his paper "THE Classic of LCAO MO Theory." A Google search on computational chemistry and Roothaan results in over 49,000 citations.

Clemens and his students from the University of Chicago Laboratory for Molecular Structure and Spectra continued over the years to produce significant contributions that advanced the state of computational chemistry. The 1993 Sanibel International Quantum Chemistry Symposium was held to honor the work flowing from Clemens and his University of Chicago group.

At the time of the Sanibel Symposium, Clemens had been hard at work as a senior scientist in Hewlett Packard Laboratories, on codes that helped set the basic parameters of the architecture we now know as Itanium. Many architecture choices were based upon the detailed codes and insights that Clemens developed. Because I had learned to program in Clemens's Lab at the University of Chicago I also had been invited to say a few words at the Sanibel Symposium. I told the audience that I looked forward to the day when I could speak publicly about the outstanding work that Clemens was then doing at HP Labs. Well, today I am happy to have the opportunity to do so, and also to recognize some of his other contributions to computing.

Clemens personally was fascinated and challenged by computers nearly as much as by mathematics, physics, and chemistry. He trained his core of programmers at the University of Chicago from scratch and by example. His teaching method was jointly to develop codes in a small group around a blackboard. At the time there were no operating systems, no compilers, and paper tape and punched cards were the media du Jour. We had to construct not only I/O and function libraries, but also programs to boot the machine, load our codes, and dump the memory when faults occurred. The team Clemens built supported both his physics laboratory and also the first computer center at the University of Chicago, for which Clemens was named Director. The team went on to build one of the first multi-computer systems, where an IBM 7040 concurrently spooled two card readers and three line printers at full speed while continuously feeding batch jobs and receiving output to/from an IBM 7094. Networked input also was established to/from a small computer in the University of Chicago Billings Hospital.

Clemens was never satisfied with mediocre work. He insisted upon the principles of simplicity, rigorous thinking, crisp problem analysis, and algorithms that employed minimum time and memory. And these principles took root in the programmers he trained.

During the early 1960s, his University of Chicago computer center team, led by an exceptionally talented graduate student mathematician named Hirondo Kuki, developed libraries of mathematical function codes with which IBM replaced all its math library codes for the IBM 7040, 7044, 7090, and 7094. IBM later contracted with the University of Chicago to produce the initial mathematical function libraries for the IBM System/360 and for subsequent extensions. Hirondo Kuki also was the first to discover the danger of the lack of a rounding guard digit for IBM System/360 long floating point computations. After publicizing the implications at the IBM SHARE users' group, IBM subsequently modified both their micro codes and their hardware to include the needed guard digit.

After Clemens reached the mandatory University of Chicago retirement age in 1988, he continued his work on physics, mathematics, and computers. At Hewlett Packard he became a member of the research team that developed the research architecture, PA-WW, which formed the technical basis for the HP/Intel Itanium partnership. Clemens's focus remained high speed numerical computing, assuring that the architecture had the needed data formats and execution resources for maximum efficiency. His codes established by concrete examples the needed numbers of registers, predicates, concurrency, and instruction repertoire. His work lent rigor to decisions that otherwise might have been taken arbitrarily.

Clemens's work subsequently resulted in a full C standard compliant vector math library, developed jointly with Sverre Jarp and CERN. Mark Smith and I both regret that a death in his family prevented Sverre Jarp of CERN from joining us here this morning. The vector math library is based both upon Clemens's leading edge mathematics and his pioneering programming practices. It achieves unprecedented performance and accuracy and is openly available to you all. It can be found on the HP web site by a Google search on VML. I have a chart summarizing the speed and accuracy of this library that I would be happy to share with any of you who are interested.

Clemens's work on the vector math library went well beyond traditional programming. He reformulated the underlying mathematics of the Chebychev polynomial approximations and Ramez optimizations of the coefficients. He has continued this definitive basic mathematics work and is both writing a book about it and speaking about it at this conference. In addition, he showed how to realize maximum instruction level parallelism on Itanium and pioneered the novel tools and programming methodology used in constructing the vector math library. He also will be speaking about this at this conference. Clemens today remains a creative innovator. We at Secure64 are proud to have him associated with us as a distinguished scientist.