Mary Ann Ruth Mansigh Karlsen (Chemist, Mathematician, and Computer Scientist)

September 12, 1932-August 28, 2024

I first heard of Mary Ann Mansigh Karlsen in March, 2017 when a former co-worker at Lawrence Livermore National Laboratory (LLNL) invited me to a presentation at the Livermore Public Library. I had a conflict of schedule so was not able to watch the presentation, but I googled her and was surprised on how much time she spent working at LLNL supporting one scientist Dr. Berni Julian Alder. Dr. Alder was famous for molecular dynamics. Molecular dynamics (MD) is a computer simulation method for analyzing the physical movements of atoms and molecules. It is a key tool for the study of condensed matter systems. Molecular dynamics is now studied in departments around the world and has revolutionized human understanding of the behavior of atoms, molecules, and solids. Mary Ann was the entire software development team of Dr. Alder. I regret that I was not able to see the presentation in person but glad I was able to watch it on YouTube.

Her science journey began when Mary Ann Ruth Mansigh was born in her grandparents' farmhouse in Otter Tail County, Minnesota, 90 miles from Fargo. Her grandparents were immigrants from Finland. Her mother was 12 years old when she arrived in America from Finland. When Mary Ann was 5 years old, her parents John and Esther Mansigh bought a 5-acre piece of land in New York Mills, Minnesota where Mary Ann said she and her two siblings Milton and Marcy spent a happy childhood despite having no running water or electricity. Mary Ann was very smart and learned to read on her own at four years old. She went to the local schools and graduated as valedictorian at New York Mills High School. At that time the State of Minnesota gave one-year scholarships at the University of Minnesota to the girl and boy who

graduated with the highest grades. She enrolled at the University of Minnesota in Duluth with the intention of getting a degree in education and teaching afterward. Most of her high school female classmates went to a two-year college so they could teach elementary school.

At the University of Minnesota, she was the only female student taking science classes. She realized that she loved math, so she took all the math classes she could get into. She finished with a bachelor's degree in education with math and chemistry as her major and physics as her minor. But after graduation, she decided that teaching was not for her. She flew to California to help her sister in Berkeley who was expecting her first child. She got a chemist job at Chlorox but she did not like it and so she kept looking for another job. Then she read an advertisement at the Oakland Tribune under the heading MEN WANTED, looking for Graduates of Mathematics at the University of California Radiation Laboratory (UCRL) at Livermore, now called Lawrence Livermore National Laboratory (LLNL). She completely ignored the "Men" part of the "Men Wanted" ad and asked her roommate who owns a car to drive her to Livermore. They arrived on a Friday afternoon when most of the employees had gone home. The head of the Computations Department had left but his assistant was still there. He interviewed her and asked her to start work the next Monday.

WORK AT UC RADIATION LABORATORY

The University of California Radiation Laboratory established its Livermore branch in 1952 as a multidisciplinary research and development center focusing on weapons development and stewardship and national security. Later its name was changed to Lawrence Livermore National Laboratory (LLNL). LLNL together with Los Alamos National Laboratory (LANL) and Sandia National Laboratory (SNL) comprise the three nuclear weapons laboratories operated by the US Department of Energy. When Mary Ann Mansigh worked there in 1955, the laboratory has only been in existence for 3 years. She was assigned to work as a human computer. Computers were mostly women working at a desk, adding thousands and thousands of numbers all day. There were three women doing that job. She was supposed to be the fourth one, but she declined. She was then assigned to study digital computers, along with 25 men. All these 25 men had come back from World War II. Most have a science background but not in mathematics. Mary Ann was the only woman and the youngest one in the group. No one knew what a digital computer was. When she first saw the UNIVAC1 (short for Universal Automatic Computer) machine, she was in awe of it! She could not believe that this machine could calculate faster than her! They were given a piece of paper with instructions about the machine. One of the guys passed by her desk, saw her totally confused and was nice enough to explain to her what to do. That was her first lesson in programming! The UNIVAC1 was the first

digital computer she worked on but not the last. She went on from UNIVAC1 to IBM 704, 709 and 7090, CDC 1604, 6600 and 7600. The last computer she worked on before she retired in 1994 was the Cray 1 computer. She basically saw the evolution of computers from the 1950's to the 1980's as a real computer pioneer.

WORKING WITH DR. BERNI ALDER AND TOM WAINWRIGHT

Mary Ann did not originally support Berni Alder. Another programmer, Mary Grace, who shared an office with Mary Ann, was supporting Berni Alder. When Mary Grace got pregnant and left the Laboratory in 1958, Mary Ann took over her job of supporting Berni Alder. Berni Alder was a German -born physicist who specialized in statistical mechanics and was a pioneer of computational modelling of matter. He and Thomas Everett Wainwright developed the techniques for molecular dynamics simulation in the mid 1950's. In particular, their techniques were used to compute the liquid-solid phase transition for a hard sphere and velocity autocorrelations function decay in liquids.

The Weapons Department was responsible for the computers at the Radiation Laboratory. But Berni Alder wasn't in that department – he was a theoretical physicist working on molecular dynamics research. So, he made an agreement with the physicists at the Weapons Department, to let Mary Ann use the computers when they were idle, i.e. not being used by the Weapons Department physicists.

She mainly supported Berni Alder's research on molecular dynamics. Mary Ann was Berni Alder's entire software development team She started using machine language programming but then switched to FORTRAN when that compiler became available. She said she started using a primitive version of FORTRAN in the 1960s and continued with more sophisticated dialects as FORTRAN developed into the 1980s.

For the remainder of her career, Mary Ann developed code for another eminent scientist, Dr. Donald Wuebbles. The work was modeling the atmosphere in order to understand the process of ozone depletion in the atmosphere and how to protect the atmospheric ozone layer. Dr. Wuebbles is currently the Harry E. Preble Emeritus Professor of Atmospheric Science at the University of Illinois. He has two degrees in Electrical Engineering from the University of Illinois and a Ph.D. from the University of California, Davis, in Atmospheric Science. After twenty years at Lawrence Livermore National Laboratory, Dr. Wuebbles went back to the University of Illinois in 1994, as Professor and Head of the Department of Atmospheric Sciences. When he left Lawrence Livermore Laboratory, Mary Ann retired.

Around 2015, Mary Ann's contributions to the field of computational physics were recognized. She was a special guest at Berni Alder's Symposium in August 2015 which celebrated Berni's 90th birthday. The Women in Science and Engineering group of the Lawrence Livermore Laboratory Women's Association invited Mary Ann to speak at a brown bag seminar. She met a new generation of LLNL women scientists and engineers who were eager to learn about her technical work and how she worked as a woman scientist at a time when there were not as many women working in the field. She then got invitations to speak from other organizations including the March 19, 2017, talk she gave at the City of Livermore Library sponsored by the Friends of Livermore Library and the American Association of University Women (AAUW), Livermore-Pleasanton-Dublin branch.

On November 15, 2017, the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and NCCR MARVEL (the Swiss center for "Computational Design and Discovery of Novel Materials") sponsored a talk by Mary Ann Mansigh at the EPFL (École Polytechnique Fédérale de Lausanne) campus in Lausanne, Switzerland. She impressed them enough that later they named a lecture series of prominent scientists from all over the world after her. The Mary Ann Mansigh Conversation series focuses on non-strictly technical topics of cultural interest for the

simulation and modelling community. The format reflects the informative and informal nature of these sessions, with talks introducing the subject followed by a conversation between the speakers and the audience. It is sponsored by CECAM, and NCCR-MARVEL.

On March 9, 2018, she was the keynote speaker for Marvell Semiconductor's International Women's Day celebration. On Aug. 25, 2024, three days before her death, she received news that she was selected for an honorary doctorate from Eidgenössische Technische Hochschule Zürich (Federal Institute of Technology Zurich, usually called ETH-Zurich).

On Aust 28, 2024 Mary Ann passed away in her sleep. She is survived by her spouse Cori Elena Karlsen whom she married after retiring.

HER LEGACY

Mary Ann Marsigh Karlsen will be remembered as a computer science pioneer and a collaborator with Dr. Berni Alder and Dr. Thomas Wainwright in developing techniques for molecular dynamics simulation in the mid-1950's including the liquid-solid phase transition for hard sphere and the velocity autocorrelations function decay in liquids. She will be remembered for the Mary Ann Mansigh Conversation Series (mamcs), a lecture series sponsored by CECAM and NCCR-MARVEL in Lausanne, Switzerland which was named in her honor. She will be remembered for being a role model for women scientists and engineers.

HER SCIENCE JOURNEY

1932 - Mary Ann Mansigh was born in Otter Tail County, Minnesota

1937 - Her family moved to New York Mills, Minnesota

1950 - Graduated valedictorian at New York Mills High School and enrolled at University of Minnesota in Duluth, Minnesota

1954 - Finished college with a bachelor's degree in education major in mathematics and chemistry and minor in physics at the University of Minnesota, Duluth.

- Moved to Berkeley, California, worked at Chlorox as a chemist

1955 - Started working at Lawrence Livermore National Laboratory and worked at UNIVAC 1-

1958 - Started supporting Berni Alder in his Molecular Dynamics project

1994 - Retired from Lawrence Livermore National Laboratory

1997 - Married Cori Elena Karlsen

2015 - Gave a talk to the Women in Science and Engineering (WISE) group at Lawrence Livermore National Laboratory

2017 - Gave a talk at the Livermore Public Library and the CECAM/MARVEL Talk in Lausanne, Switzerland

2018 - Keynote speaker for Marvell Semiconductor's International Women's Day Celebration

2019 - The Mary Ann Mansigh Conversation Series had its inaugural speaker, Massimo Noro of Daresbury Laboratory in the United Kingdom. His talk was about computer modelling for industrial applications

2024 - Mary Ann was selected for an honorary doctorate from Eidgenössische Technische Hochschule Zürich (Federal Institute of Technology Zurich) on August 25th.

- Passed away in her sleep on August 28th.

BIBLIOGRAPHY

Since there are no books written about Mary Ann Mansigh Karlsen, I relied on the information on her obituary from the Independent Newspaper, the local newspaper in Livermore and also the obituary posted at Lawrence Livermore National Laboratory's website. I watched the video of her talk at the Livermore Public Library and the CECAM-NCCR MARVEL talk given in Lausanne, Switzerland.

The information and photos were taken from the following websites:

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