

Excerpt from an email exchange between Herman Berendsen and Giovanni Ciccotti, 15 June 2017

GC When did you start thinking of doing MS, in particular, immediately or in a second moment to study proteins (more generally biological matter)?

HB I started out as an experimentalist. My thesis research (1959-1962) was on nuclear magnetic resonance of biological material, in order to find out the details of water organisation in biological tissue. I put all kinds of living and dead biological tissue in the (then new) NMR machines, which were then being developed to measure water content and organisation. I found that hydrated tendon (which I got from the local butcher) showed a line splitting dependent on the orientation in the magnetic field. Later I used rat tail tendon, which consists of nicely oriented collagen fibers. A rather pure system, which showed that water molecules were on the average oriented with respect to the collagen fibers. The observed dipole splitting could be well explained by the binding pattern of fluctuating hydrogen bonds between water and groups on the collagen polypeptide.

When writing my thesis about this in 1962, I wondered if such a simple property as average orientation of water molecules could not be computed, even with the then available, limited computational facilities and knowing the basic interactions between water molecules and substrate atoms, just by mimicking atomic motions. That is, by molecular dynamics, but that name did not yet exist. The more fundamental question was: can we simulate the motion of water molecules in the liquid state?

My job then, as associate professor in physical chemistry, gave me every opportunity to pursue this idea. I also met Carl Moser around that time, who persuaded me to organise a CECAM summer workshop on "MC and MD of water" in Orsay. I contacted several people and the workshop took place in 1972. One of the most influential participants from whom I learned most, was Aneesur Rahman. In the [CECAM "in memoriam" publication](#) after Rahman's death in 1987, I gave a review of my contacts with Anees and other CECAM activities on page 6-13.