On Some Additional Recollections, and the Absence Thereof, about the Early History of Computer Simulations in Statistical Mechanics

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On Some Additional Recollections, and the Absence Thereof, about the Early History of Computer Simulations in Statistical Mechanics *

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When Professor Ciccotti asked me to speak again on the early history of computer simulations in statistical mechanics, I was rather reluctant to do so, for the reason that most of what I can reliably report has already been written in the paper [1] that I presented ten years ago at "Corso 97" in Varenna. But the pleasant prospect of once again visiting this beautiful country, as well as learning about a lot of interesting work, overcame my distaste for repeating things that I have said or written before. Nevertheless, while there may be some merit in repeating some of the material in a lecture presented to a different and, in part, younger group, in this written summary I will for the most part confine myself to extending and correcting, where necessary, the previous account.

I must again begin by emphasizing, as regards my own role in this early history, that it was exclusively with applications of the Metropolis Monte Carlo method. And even there, I became involved only after the preparation of both the seminal paper by Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller [2] and the subsequent paper by Rosenbluth and Rosenbluth [3]. I by no means claim any part in the invention of the method.

With regard to the molecular dynamics method, my only connection with the early work was my collaboration with Alder and Wainwright in our joint effort to reconcile the results of the Monte Carlo and molecular dynamics methods for hard spheres\(^1\). My Varenna paper recounts that collaboration in considerable detail. I again emphasize in the strongest possible terms that in that account I did not rely on my memory of those long-ago events, but rather on files in my possession of the correspondence between Alder and me, and between Kirkwood and me, as well as monthly progress reports of our work at Los Alamos which are on file at the Los Alamos National Laboratory. I had always regarded that collaboration as a very pleasant one. Thus I was utterly dismayed to read the following in a recent paper by Alder [4]:

"But by that time, some years later, Bill Wood at Los Alamos had gone so far in the Monte Carlo calculations that I said 'Well, we must try to do something else', particularly since he had not found the hard sphere phase transition by the Monte Carlo method."

And later:

\(^1\)Throughout this paper, the term "hard spheres" refers to the three-dimensional case; I use "hard disks" for the two-dimensional case.
“In that paper [WWW: the reference is to [5]], there was already the velocity autocorrelation function decay, but, of course, it did not have enough numerical resolution. So then we went back to our first love which was the hard sphere transition. I had to know whether Bill Wood had done his job right by Monte Carlo and it turned out that he had not. By molecular dynamics we found a phase transition and subsequently Wood also found it and that’s a long story.”

These quotations are a miserable distortion of what actually happened! As I mentioned in [1], I began my work with the Metropolis Monte Carlo method by applying it to systems of Lennard-Jones particles, in the belief that the Rosenbluths [3] had done as much as was feasible for hard spheres with the computing resources of that era. Recently, while looking through my surviving notes from this time, I discovered that we did check our new code against their results by doing a calculation for hard spheres, but we happened to choose a density well above the transition region, and indeed got a result satisfactorily close to theirs. It was not until Alder told me about his difficulty in reproducing the Rosenbluth results for the hard sphere equation of state by means of molecular dynamics that, at Alder’s request, my associates and I undertook a re-investigation by means of the Metropolis method. The chronology of the resulting collaboration between the Livermore and Los Alamos groups is given in [1]. I am greatly disappointed that Alder remembers it differently. Questions of priority do not greatly interest me, but as far as which of the two methods first saw indications of the hard sphere phase transition is concerned, interested persons should read my Varenna paper, as well as the exchanges between Kirkwood and Alder in the verbatim transcripts of the two round table discussions at the 1957 Stevens Institute symposium [6]. I would emphasize that these early results only suggested, but by no means proved, the existence of a first-order phase transition in the thermodynamic limit, since the calculations at that time were limited to quite small systems.

In reading through my paper of ten years ago in preparation for this talk, I was struck by the need to correct it in one respect, and to amplify it in another.

First, I realized that one could easily come away from it with the impression that Professor Kirkwood, my mentor (of whom I have only the fondest memories), was completely unjustified in his objections to the proofs of the correctness of the Metropolis method that were given in [2], [3], and the
unpublished paper by Rosenbluth that I mentioned in [1]. That is not the case. Briefly, he was soon able to agree that those arguments made it at least plausible that the method would correctly generate the canonical distribution when applied to an ensemble of N-body systems. But he rightly objected that the argument, that averaging over a single such system would yield the canonical average, was very weak.

Second, a point which needs some amplification was suggested by a question asked by Professor Ciccotti: Namely, when did we discover that the Metropolis method consists in the generation of a realization of a Markov chain, for which there was a large body of mathematical theory that made the justification of the method quite a simple matter? As far as I am aware, the first publication mentioning that fact is my 1957 paper with Parker [7]. The papers of Metropolis, et al. [2] and the Rosenbluths [3] make no mention of Markov chains, which in retrospect seems a bit odd in that the 1949 paper by Metropolis and Ulam [8] mentions them in passing. As I mentioned in [1], most of my notes on the early work, including the preparation of the 1957 paper, long ago fell victim to bureaucratic enthusiasm for the destruction of files. I do remember very clearly the following event, though not when it occurred. One day I met Marshall Rosenbluth in a hallway. He mentioned that he had been browsing in a book on probability theory, which he had noticed in the new book display in the library. He suggested that I take a look at the chapter on Markov chains, as he suspected that they had something to do with the method. At that point I knew nothing about Markov chains, as I had never had a course in probability theory, or for that matter, one in statistics. The book was the one by Feller [9] which we cited in our 1957 paper. I don’t remember how long it took, but soon everything became quite clear. When did this occur? Reasoning from the absence of any mention of such a discovery in my correspondence with Kirkwood through April 1954, when we were arguing about the validity of the method, as well as in the above-mentioned series of reports, which began in September 1954, my best guess is that our acquaintance with Markov chains began between April and September 1954. But it could have been earlier, in which case it must have been described to Kirkwood in the course of conversations with him, rather than in correspondence.

Finally, in the few remarks that I made about hard disks in [1], I should have taken note of the large number of investigations that have been stimulated by the two-dimensional melting theories of Halperin and Nelson [10], and of Young [11]. Those theories predict that the transition is not first-order, but instead that it consists of two second-order transitions with an
intervening "hexatic" phase. There is an extensive review, with references through 1987, by Strandburg [12]. More recent Monte Carlo investigations have been carried out by Zollweg and Chester [13] and by Lee and Strandburg [14]. Both investigations find the transition to be more weakly first-order than found in the early work of Alder and Wainwright [15], with Zollweg and Chester noting that it is possible that the transition might even become of higher order in the thermodynamic limit. It is quite interesting, and perhaps even surprising, that the question still remains unsettled almost forty years after the early work of Alder and myself.
References


[4] B. J. Alder, in Microscopic Simulation of Complex Hydrodynamic Phenomena, edited by M. Mareschal and B. L. Holian (Plenum, 1992), pp. 425-430. Alder has informed me that this paper is a transcript of taped remarks which he did not have an opportunity to edit before publication.


