In retrospect

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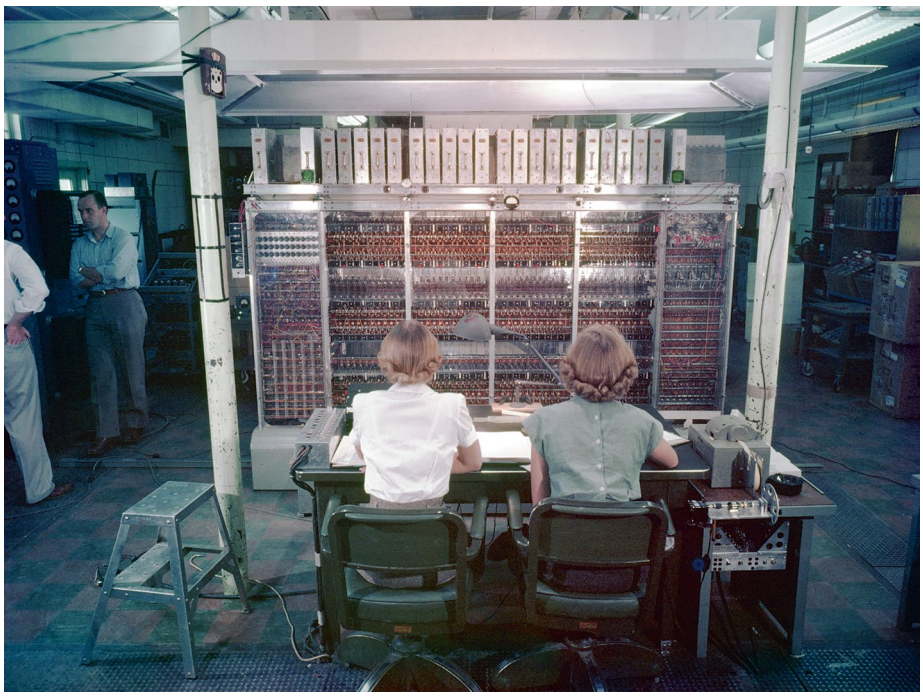
The early days of Monte Carlo methods



"The purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules." This is, in a nutshell, a 1953 article by Nicholas Metropolis, Arianna and Marshall Rosenbluth and Augusta and Edward Teller. The paper, published in the *Journal of Chemical Physics* introduced the ideas behind the celebrated Metropolis – later known as Metropolis–Hastings – algorithm, a widely-used Markov chain Monte Carlo sampling method. And while its scientific legacy is broadly appreciated, the 'behind the paper' story is less known.

On the 50th anniversary of the paper, Marshall Rosenbluth gave a personal account of how it came about. It was 1949–1952 at Los Alamos and two physicists couples, the Rosenbluths and the and Tellers, were among the scientists frantically working on the development of the hydrogen bomb proposed by Edward Teller. Understanding the interactions between radiation and matter at extreme conditions was key for the bomb design and it required complex calculations that, until the end of 1951, were done analytically or using IBM punch-card machines.

Meanwhile, Metropolis was busy with the construction of a machine like the one John von Neumann had built at the Institute for Advanced Study at Princeton. Metropolis's computer called MANIAC (the acronym standing for Mathematical Analyzer Numerical Integrator and Automatic Computer, or, as physicist George Gamow humorously suggested, for Metropolis And Neumann Invent Awful Contraption) started running at Los Alamos in 1952. Marshall Rosenbluth enlisted the help of the Tellers and convinced Metropolis to give them the midnight shift on MANIAC (pictured).

The Rosenbluths were studying the equation of state based on the two-dimensional motion of hard spheres. "Of course, our first thought was straightforward molecular dynamics", recalled Marshall Rosenbluth, but "it looked impossible to use an adequate number of particles with the MANIAC's limited capabilities." Then, Edward Teller suggested to make use of statistical mechanics and take ensemble averages instead of following detailed kinematics. They knew that Stanislaw Ulam had come up with the idea that instead of considering all possible trajectories one could rather take a random sample, an idea enthusiastically endorsed by von Neumann. But such a Monte Carlo approach – a term coined by Metropolis – required a powerful computer. With time available on the MANIAC, Arianna Rosenbluth "coded the algorithm up within the limits imposed by machine capability" (likely with Augusta Teller) and the algorithm turned out to work extremely well.

Marshall Rosenbluth's account is remarkable in several ways. It reveals both the ironically minor role Metropolis played in this landmark paper and the major, previously unknown, contribution of Arianna Rosenbluth. Their work is also one of the earliest examples of algorithms designed specifically for an electronic computer. 70 years on, the paper reads very modern and is perhaps among the first computational physics articles ever written.

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Original article: Metropolis, N. et al. Equation of state calculations by fast computing machines. *J. Chem. Phys.* **21**, 1087–1092 (1953)

Related articles: Rosenbluth, M. N. Genesis of the Monte Carlo algorithm for statistical mechanics. *AIP Conf. Proc.* **690**, 22–30 (2003); Wells, M. B. In *Computing at LASL in the 1940s and 1950s* 16–21 (LANL, 1978); https://doi.org/10.2172/6611027; Metropolis, N. & Ulam, S. The Monte Carlo method. *J. Am. Stat. Assoc.* **44**, 335–341 (1949)