The origin of computational Statistical Mechanics in France

D. Levesque, J. Hansen

The origin of computational Statistical Mechanics in France

D. Levesque[1,a] and J.P. Hansen[2,3]

[1] Laboratoire de Physique Théorique Bâtiment 210, Université Paris-Saclay, 91400 Orsay, France
[2] Laboratoire Phénix, Université Pierre et Marie Curie, 75005 Paris, France
[3] Department of Chemistry, University of Cambridge, Cambridge CB2 1EW, United Kingdom

Abstract. The two main methodologies of computational Statistical Mechanics, namely the stochastic Monte Carlo and the deterministic Molecular Dynamics methods, were developed in the USA in the mid nineteen fifties. In the present paper we show how these "computer experiments" migrated to Europe in the sixties, and first bloomed at the Orsay Science Faculty, before spreading throughout Europe. Collaborations between the Orsay group, led by Loup Verlet, and pioneering groups in the USA and Europe are pointed out. Finally it is shown how the celebrated Verlet algorithm for the integration of classical equations of motion can be traced back to Isaac Newton.

1 Introduction

The basic principles of Statistical Mechanics were established during the second half of the nineteenth and the beginning of the 20th century by Maxwell, Boltzmann and Gibbs. Exact results for the thermodynamic properties of many-particle systems could be derived analytically for some simple models, culminating in the solution of the two-dimensional Ising model by Onsager [Onsager 1944]. However very few models have analytic solutions, so that approximations, like mean-field, must be made to predict thermodynamic, structural or transport properties of physically relevant models.

This situation changed radically with the appearance, during and after World-War II, of the first electronic computers which were mostly based, for defence reasons, at the US National Laboratories at Los Alamos and at Livermore. This led to the development of numerical simulation methods for classical many-particle systems, namely the Metropolis Monte-Carlo (MC) method [Metropolis 1953, Rosenbluth 1955, Wood 1957a] and the Molecular Dynamics (MD) method [Alder 1957, Alder 1959]. The initial MD code of Berni Alder and Tom Wainwright, assisted by Mary Ann Mansigh, was designed for hard disks (in 2d) or hard spheres undergoing elastic binary collisions. The extension to systems interacting via "soft", continuous pair potentials was later put forward by Anees Rahman at the Argonne National Laboratory [Rahman 1964]. The early MC and MD simulations led immediately to a major, unexpected discovery, namely the purely entropy-driven

[a] e-mail: dominique.levesque@u-psud.fr

freezing of hard disks and spheres at sufficiently high packing fractions [Alder 1957, Wood 1957b].

The pioneering period of computational Statistical Mechanics is well described in a recent paper by Michel Mareschal [Mareschal 2018]. In the present paper we report how computational Statistical Mechanics was imported to Europe, and more specifically to France, where the first group developing "computer experiments" worked at the Orsay Faculty of Science. In Section 2 we follow the emergence of a computational Statistical Mechanics group within the newly founded Laboratory of Theoretical Physics and High Energies at Orsay in the late 1950's. Section 3 describes the context of the development of MD and MC at Orsay throughout the sixties and beyond. Prolongations and the diversification of these computational activities are analysed in Section 4, while in the Conclusion we report the link between the most commonly used MD algorithm for the integration of the equations of motion and a Theorem due to Isaac Newton!

2 The Orsay Statistical Physics group

In 1960, the Orsay Science Campus (located 20 km south of Paris), still part of the Faculty of Science of the University of Paris (Sorbonne), is in a phase of rapid development. Several buildings are under construction, to host new laboratories, in particular the "Laboratoire de Physique Théorique et Hautes Énergies" (LPTHE). From the onset, its founder and director, Professor Maurice Lévy, wished the LPTHE to be multi-disciplinary, bringing together theoreticians of elementary particles physics, nuclear physics, statistical physics and mathematical physics. In these early days, LPTHE numbered about 20-30 scientists, including PhD students, and occupied half a floor of the freshly built "211" building, which also hosted solid-state and plasma physics laboratories.

The statistical physics group was led by Loup Verlet, a "transfuge" from elementary particle and nuclear physics [Drell 1955]. In 1959, he derived the hyper-netted-chain (HNC) equation [Verlet 1960], simultaneously and independently of other authors, using a diagrammatic re-summation method, a highly "fashionable" exercise at that time. The HNC equation, as well as the Percus-Yevick (PY) equation derived around the same time [Percus 1958] are approximate closure relations which supplement the Ornstein-Zernike relation between total and direct pair correlation functions [Ornstein 1914]. These integral equations were at the basis of theoretical developments in statistical physics of dense fluids and liquids throughout the sixties and beyond.

While the PY equation admits an analytic solution for the case of a hard sphere fluid [Thiele 1963, Wertheim 1963, Baxter 1968], no such solutions exist for the HNC equation, nor for more "realistic" models, like the Lennard-Jones (LJ) pair potential, of real fluids, within either PY or HNC. It is hence clear that one had to resort to numerical solutions of these integral equations in order to allow a quantitative comparison of the predictions of these approximate theories with experimental data.

In that perspective, the statistical physics group at LPTHE was to benefit from the creation by Maurice Lévy and Loup Verlet, with the support of other laboratories, of the computing centre of the Orsay Faculty. The computer which was installed in building 211, was one of the first commercially available machines in the world, namely the IBM 650. The central processor unit still used vacuum tubes, like radio sets of that period! The central memory of 2000 words of ten decimal digits was located on a magnetic drum which rotated at the frequency of several thousand revolutions per minute and contained both instructions and data. The execution time of instructions

and arithmetic operations was of the order of a millisecond. Programming was preferentially in machine language, each elementary operation being coded on punched cards. Shortly thereafter a second machine was installed at Orsay Faculty, namely a CAB 500 computer built by SEA (Société d'Électronique et d'Automatisme) company. This machine had a magnetic drum memory of 16000 words of 10 digits; the typical execution time of arithmetic operations was of the order of 40 milliseconds.

Loup Verlet and his PhD student Dominique Levesque used mainly the IBM 650 to get acquainted with calculations on a computer. They developed programs to solve the HNC and PY equations by an iterative method carried out in real space since the Fourier transformation did not provide any advantage within the IBM 650 architecture and its Fast Fourier version [Cooley 1965] clearly not adapted to decimal arithmetics.

Meanwhile the seminal papers of the MC and MD methods by Metropolis et al., Rosenbluth and Rosenbluth, Wood and Parker and Alder and Wainwright already quoted, had not escaped the attention of the statistical physics group of LPTHE and were studied in detail by the Verlet group. The results of these papers, in particular those of Alder and Wainwright for hard spheres, allowed an appreciation of the quantitative validity of the PY and HNC equations for that system. A similar comparison with experimental data for rare gases also provided such an appreciation, which is however less reliable because of the uncertainty of the interatomic interaction modeled by the LJ pair potential. In view of these comparisons, improvements of the PY and HNC equations were put forward by the Verlet group. Functional expansions were used to derive corrections to the PY equation, while an attempt was made to improve the HNC closure by including some so called "bridge" diagrams neglected within HNC [Verlet 1964, Verlet 1965]. It is for computing the simplest bridge diagram that the Verlet group used for the first time the MC method [Verlet 1962].

In 1965-1966, Loup Verlet was invited by Joël Lebowitz to spend one year at the Belfer Graduate School in New-York. This was the year after the publication of the seminal paper by Anees Rahman on the MD simulation of a system of particles interacting via the LJ pair potential [Rahman 1964]. Loup Verlet who had noticed this article before his departure for the US, decided to extend Rahman's pioneering work along several lines. First, Lebowitz, Percus and Verlet established that, since a time average taken within the course of a MD simulation, at constant total energy and momentum, is equivalent to a micro-canonical average, all thermodynamics quantities can be computed from the time evolution of the dynamical variables themselves or their fluctuations [Lebowitz 1967]. For instance, the time average of the kinetic energy fluctuations allows the calculation of the system's specific heat. Next, on an up-to-date CDC computer newly accessible at the Courant Institute of New-York University, Loup Verlet implemented a MD code innovating along two lines, namely an algorithm for the integration of the Newtonian equations of motion and the awareness of the range of the molecular and atomic interactions [Verlet 1967]. These fundamental innovations are now universally acknowledged and used.

Concerning the second point, the work on the HNC and PY equation had shown that the asymptotic decay of the LJ potential could be accounted for by assuming that at large distances the pair distribution function is equal to its asymptotic value $g(r \to \infty) = 1$. Verlet exploited this observation in his MD code by using appropriate near neighbour tables around each particle, optimally up-dated to account for the relative motion of the N particles. This procedure is easily validated by comparing the results obtained with these tables to simulations taking into account all $N(N-1)/2$ pairs of particles. The tables allow the simulation of much larger systems, since the computation time becomes of the order $N \ln N$ rather N^2. In Verlet's initial implementation [Verlet 1967] for a system of 864 particles, the simulation time, for comparable statistical errors, was reduced by more than a factor of 4.

Concerning the integration algorithm, Verlet replaced the somewhat cumbersome Runge-Kutta algorithm used by Anees Rahman by the appealingly simple algorithm:

$$\overrightarrow{\boldsymbol{r}}(t+dt) = 2\,\overrightarrow{\boldsymbol{r}}(t) - \overrightarrow{\boldsymbol{r}}(t-dt) + dt^2\,\overrightarrow{\boldsymbol{f}}(t)/m \tag{1}$$

where $\overrightarrow{\boldsymbol{r}}(t)$ is the position of a particle with mass m at time t and $\overrightarrow{\boldsymbol{f}}(t)$ is the total force acting on the particle at time t. The algorithm is obviously reversible and valid to order dt^4.

The original MD program was written by Verlet in Fortran II CDC. On his return from New-York, it was immediately transcribed on the new computer installed in Orsay: the Univac 1107, followed by the Univac 1108. The latter was, during the period 1967-1970, one of the most powerful commercially available computers. The execution times of arithmetic operations were of the order of few microseconds, while the operating system was among the first multi-tasking. Engineers from IBM-France came to Orsay to observe *de visu* this functionality which is now standard!

The early MD runs sparked a number of questions concerning the size of the simulated systems and the rigour with which the conservation laws had to be satisfied. The non-conservation of the momentum was the simplest case, since it results exclusively from the choice of initial conditions and the round-off errors affecting the calculation of the forces. Regarding the latter, the Univac 1108 had the advantage of coding floating point numbers with 36 bits (rather 32 on IBM). Moreover the Verlet algorithm Eq. (1) is independent of particle velocities, the latter being only required for the calculation of the total energy and the temperature via:

$$\overrightarrow{\boldsymbol{v}}(t) = \frac{\overrightarrow{\boldsymbol{r}}(t+dt) - \overrightarrow{\boldsymbol{r}}(t-dt)}{2\,dt} \tag{2}$$

The integration time step was chosen empirically to ensure energy conservation within a relative error $10^{-3} - 10^{-4}$ over runs of several thousand time-steps after equilibration. Simulations were generally run at night or during week-ends by members of the Verlet team so as to benefit from favourable financial conditions, and to avoid delaying the calculations of other users.

While the team had full confidence in the validity of the calculated thermodynamic and structural quantities due to the equivalence between time average, computed by MD simulation at constant energy, and micro-canonical average, questions arose on the precision to be achieved on the particle trajectories for a realistic estimate of the time-dependent correlation functions, like the velocity autocorrelation functions. In the late sixties, the importance of accounting for the conservation of the phase space volume had not yet been clearly recognized. In particular the fact that Anees Rahman's algorithm is not symplectic, while the Verlet algorithm Eq. (1) is, had not yet been noted.

It was hence on the basis of the equivalence, anticipated by Boltzmann, between MD and the micro-canonical ensemble, combined with a heuristic implementation of practical details that the use of MD flourished at the LPTHE in Orsay. It was, of course, recognized both at Orsay and elsewhere, that a MD program is readily transformed into a MC program at the cost of a few minor modification and the inclusion of a subroutine providing a truly reliable random number generator.

In particular, independently of the seminal Quantum Monte Carlo (QMC) paper by W.E. McMillan [McMillan 1965], Verlet and his students used the formal analogy between a Jastrow trial wavefunction [Jastrow 1955] and the Boltzmann factor for a system of N classical pair-wise interacting particles, to calculate the ground-state energy of liquid He_4 [Levesque 1965]; the preprint remained unpublished because McMillan's paper appeared in print just as the Orsay preprint was completed. The

preprint was later supplemented by a paper on the ground state of He_4 and He_3, using a Jastrow-Slater wave-function for the fermion case, written by D. Schiff and L. Verlet while both were in New-York [Schiff 1967]. At about the same time, back in Orsay, J.P. Hansen and D. Levesque used a Jastrow wave function, multiplied by a product of Gaussians centered on the crystal lattice positions, within a variational QMC calculation, to determine the ground-state energies of solid He_4 and He_3 [Hansen 1968]. These investigations of the ground states of liquid and solid Helium, based on variational approaches, were extended in 1973 - 74 within the framework of a collaboration with Mal Kalos. Kalos had initiated and promoted a ground-breaking Monte-Carlo method allowing the exact sampling of the ground-state wavefunction of many-boson systems, referred to as Green's Function Monte-Carlo. The collaboration led to the first application of this exact algorithm to an N-body system, namely a quantum system of hard spheres [Kalos 1974].

3 The context of the development of MD and MC at Orsay: the late sixties and beyond

The development of MD and MC simulations at LPTHE in the sixties and early seventies was based on the close collaboration of Loup Verlet with his students: Dominique Levesque, Daniel Schiff, Jacques Vieillard-Baron, Jean-Pierre Hansen, and Jean-Jacques Weis and the mutual collaboration of group members. Verlet's group also benefited from a very active international collaboration with distinguished visitors including: Berni Alder, Anees Rahman, John Valleau, Ian Mc Donald, Konrad Singer, Mal Kalos, George Stell, Mark Nelkin and post-docs Juhani Kurkijarvi, Roy Pollock among others.

In the academic research environnement of France during the sixties and early seventies, the simulation work of the LPTHE group was favourably regarded as witnessed by the Langevin prize of the French Physical Society awarded to Loup Verlet in 1971. At this time, it was clear that MD and MC simulations applied to simple classical or quantum systems were able to establish the limits of validity of approximate theoretical approaches, and even to predict unexpected physical phenomena like the freezing of hard spheres or the algebraic (rather than exponential) decay of time dependent correlation functions [Alder 1967, Levesque 1974]. But it was much less clear that these simulation methods would eventually be able to study genuinely complex systems, just as it was difficult to foresee the near exponential growth of computer power, at exponentially decreasing costs, which we have been witnessing in the last decades.

Meanwhile, strengthening the development of the Orsay Faculty, the Centre National de la Recherche Scientifique (CNRS) established on the Orsay campus, at the end of the sixties, the Centre Inter-Régional de Calcul Électronique (CIRCÉ), a national computational facility equipped with an IBM computer. However at the LPTHE, the coding of the MD and MC programs which was partly in Univac machine language, in order to reduce computational times, prevented an immediate portability of the codes to other computers. Moreover, since the installation of the Univac computers at Orsay had hardly been welcomed by IBM, the LPTHE group had developed a kind of "allergy" towards IBM, and used the CIRCÉ facilities only very marginally. Within the CIRCÉ building, Carl Moser, a quantum chemist, created the Centre Européen de Calcul Atomique et Moléculaire (CECAM) in october 1969. Members of the Verlet group did not participate, due to initial misunderstandings and the aforementioned "allergy" to IBM, in the workshops organized by CECAM which contributed strongly to the development of MD and MC methods and their

applications throughout Europe. But this initial "boycott" did not affect scientific collaborations between LPTHE group and participants of the workshops who regularly visited the LPTHE and spent sabbatical leaves with the Verlet group.

While the Orsay group focused mostly on improving and exploiting Molecular Dynamics methodologies, the Monte Carlo method in Statistical Mechanics spread simultaneously to other European countries. At Royal Holloway College near London, Ian McDonald and Konrad Singer introduced the very efficient "histogram reweighting" method [McDonald 1967], and applied it to classical fluids. In Austria, at the Technical University of Vienna, Kurt Binder applied MC sampling to discrete spin systems, in an effort to model magnetic materials and analyse neutron scattering data [Binder 1968]. At the Munich Technical University, Dietrich Stauffer was the first to use MC methods to study particle percolation on a lattice, which later led to a well-known monograph [Stauffer 1985]. More generally throughout the seventies, participants in CECAM workshops started new computational statistical mechanics groups throughout Europe, including Giovanni Ciccotti in Rome and Herman Berendsen in Groningen among others.

4 Some prolongations

In the late sixties, and early seventies, the MD and MC simulation projects at LPTHE diversified along several lines, of which we give a few examples. Daniel Schiff used "computer experiments" to investigate simple liquid metals based on effective ion-ion potentials [Schiff 1969]. Jacques Vieillard-Baron was the first to simulate assemblies of hard ellipses as a simple model for two dimensional nematic ordering [Vieillard-Baron 1972]; his pioneering work inspired the seminal papers by Daan Frenkel and collaborators on the phase diagram of lyotropic liquid crystals [Frenkel 1985]. Jean-Jacques Weis joined forces with Berni Alder and Berkeley experimentalist Herbert Strauss to investigate depolarized light scattering via MD simulations [Alder 1973]. Dominique Levesque and collaborators were the first to extend MD to simple models of rigid diatomic molecules [Barojas 1973]. Jean-Pierre Hansen joined forces with Ian Mc Donald and Roy Pollock to investigate the static and dynamical properties of the "one component plasma" (OCP) a model for highly compressed plasmas generated in inertial confinement fusion experiments, both by MC [Hansen 1973] and MD [Hansen 1975] simulations. The Verlet group also engaged in a fruitful collaboration with LPTHE theoretical physicists, in particular with Bernard Jancovici, a former classmate of Loup Verlet at École Normale Supérieure [Hansen 1972].

Around 1974, Loup Verlet and Daniel Schiff moved to other areas of research and human endeavour. In 1974 they published an opinion column in the November issue of the journal La Recherche [Verlet 1974], putting forward their questioning of the objectives of fundamental research in theoretical physics and their motivations to contribute to other areas. Their concerns, in particular those related to ecological issues are still of crucial relevance today. Loup Verlet's practice of theoretical physics also led him to an epistemological analysis of the creation and development of scientific theories published in his two books "La Malle de Newton" [Verlet 1993] and "Chimères et Paradoxes" [Verlet 2007].

5 Conclusion

To conclude this brief historical review of the development of the MD and MC simulations at Orsay Faculty, we quote an extract from Loup Verlet's book "Chimères et

Paradoxes", on pages 174-175, where Loup Verlet gives his personal account of this period:

« Immediately after World War II, the increase in power of computers allowed to reconsider the basis of the question raised by the atomistic hypothesis and addressed by Maxwell and Boltzmann in the 19th century: how to determine the macroscopic properties of gases and liquids, knowing that they are composed by large numbers of atoms obeying Newton's equations of motion and assuming that they interact via a given force law? This question became all the more pressing towards the end of the century, in light of growing evidence that atoms and molecules really exist. Until the end of the World War II, this question remained essentially unsolved except in the case of low density gases. The situation changed in the fifties due to the advancement of powerful computers. It became possible to follow, over a sufficiently long time span, the trajectories of several tens or even hundreds of particles behaving like billiard balls. A few years later it became feasible to tackle a more realistic model, namely about one thousand particles interacting via pair-wise Lennard Jones forces. Within a collective research effort, I suggested, among other procedures to speed up the calculations, a new algorithm for the integration of Newton's equation of motion of the dynamics of the molecules. Simple, stable and accurate, this algorithm can be used to simulate the motion of very complex molecules. At that time, I did not realise that the algorithm I had suggested was nothing but the generalization of the geometric algorithm of Newton ... ».

In Fig.1, we show this geometric algorithm extracted from Newton's "Principia" [Newton ed. 1883]: The particle's discrete trajectory $\overrightarrow{\boldsymbol{r}}(t)$ is the broken line A, B, C, D, E, F, ... and the source of the force acting on the particle is at S. As Loup Verlet notes on page 124 of "Chimères et Paradoxes", even if « the translation of proportionality ratios into vector equalities is anachronistic, it reflects Newton's indications », (cf. [Principia Translation 1934]). In particular the AB segment can be interpreted as $\overrightarrow{\boldsymbol{v}}(t-dt)\,dt$ or $\overrightarrow{\boldsymbol{r}}(t)-\overrightarrow{\boldsymbol{r}}(t-dt)$, the segment BV as $\overrightarrow{\boldsymbol{f}}(t)\,dt^2/m$, etc. This translation into vectorial quantities, and noting that ABCV is a parallelogram, leads to the relation:

$$[(\overrightarrow{\boldsymbol{r}}(t+dt)-\overrightarrow{\boldsymbol{r}}(t))-(\overrightarrow{\boldsymbol{r}}(t)-\overrightarrow{\boldsymbol{r}}(t-dt))]/dt^2=\overrightarrow{\boldsymbol{f}}(t)/m \tag{3}$$

which is precisely Verlet's algorithm (1).

Acknowledgements

This paper is dedicated to Loup Verlet, the central actor in our presentation, who was our mentor and thesis supervisor in the sixties. We are grateful to Giovanni Ciccotti, Gianni Battimelli and Rodolphe Vuilleumier, who organised a very fruitful workshop in Paris, bringing together computational scientists and historians of science in May 2018.

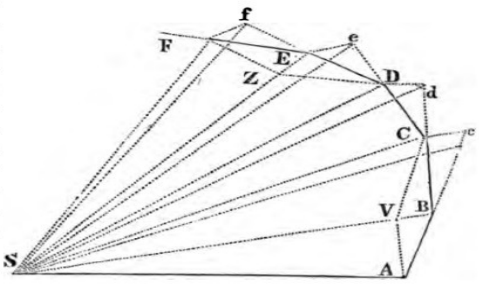
SECTIO II.

De Inventione Virium Centripetarum.

PROPOSITIO I. THEOREMA I.

Areas, quas corpora in gyros acta radiis ad immobile centrum virium ductis describunt, et in planis immobilibus consistere, et esse temporibus proportionales.

Dividatur tempus in partes æquales, et primâ temporis parte describat corpus vi insitâ rectam A B. Idem secundâ temporis parte, si nil impediret, rectà pergeret ad c, (per leg. 1.) describens lineam B c æqualem ipsi A B; adeò ut radiis A S, B S, c S ad centrum actis, confectæ forent



æquales areæ A S B, B S c. Verùm ubi corpus venit ad B, agat vis centripeta impulsu unico sed magno, efficiatque ut corpus de recta B c declinet et pergat in rectâ B C. Ipsi B S parallela agatur c C, occurrens B C in C; et completâ secundâ temporis parte, corpus (per legum Corol. 1.) reperietur in C, in eodem (*) plano cum triangulo A S B. Junge S C; et triangulum S B C, ob parallelas S B, C c, æquale erit

(*) 171. Reperitur in C, in eodem plano cum triangulo A S B; nam diagonalis B C, quam viribus conjunctis mobile describit, est in plano parallelogrammi V B c C, cujus latera B V, B c, viribus separatis describenda, sunt in plano trianguli A S B.

Fig. 1. From a facsimile edition of Newton's Philosophiae naturalis principia mathematica, schema of a particle trajectory submitted to a central force [Newton ed., 1883], cf. text below.

References

Alder B.J. and Wainwright T.E. 1957. Phase Transition for a Hard Sphere System. *J. Chem. Phys.* **27**: 1208-1209.

Alder B.J. and Wainwright T.E. 1959. Studies in Molecular Dynamics. I. General Method. *J. Chem. Phys.* **31**: 459-466.

Alder B.J. and Wainwright T.E. 1967. Velocity Autocorrelation for Hard Spheres. *Phys. Rev. Lett.* **18**: 988-990.

Alder B.J., Weis J.J. and Strauss H.L. 1973. Depolarization of Light in Atomic Fluids. *Phys. Rev. A* **7**: 281-284.

Barojas J., Levesque D. and Quentrec B. 1973. Simulation of Diatomic Homonuclear Liquids. *Phys. Rev. A* **7**: 1092-1105.

Baxter R.J. 1968. Ornstein-Zernike Relation for a Disordered Fluid. *Aust. J. Phys.* **21**: 563-569.

Binder K. and Rauch H. 1968. Calculation of spin-correlation functions in a ferromagnet with a Monte Carlo method. *Phys. Lett. A* **27**: 247-248.

Cooley J.W. and Tukey J.W. 1965. An algorithm for the machine calculation of complex Fourier series. *Mathematics of Computation* **19**: 297-301.

Drell S.D. and Verlet L. 1955. Multiple Scattering Corrections in $\pi^{\pm}$ Deuteron Scattering. *Phys. Rev.* **99**: 849-857.

Frenkel D. and Mulder B. 1985. The Hard Ellipsoid of Revolution Fluid: I. Monte-Carlo Simulations. *Mol. Phys.* **55**: 1171-1192.

Hansen J.P. and Levesque D. 1968. Ground State of Solid Helium-4 and -3. *Phys. Rev.* **165**: 293-300.

Hansen J.P., Jancovici B. and Schiff D. 1972. Phase Diagram of a Charged Bose Gas. *Phys. Rev. Lett.* **29**: 991-995.

Hansen J.P. 1973. Statistical Mechanics of Dense Ionized Matter. I. Equilibrium Properties of Classical One-component Plasma. *Phys. Rev. A* **8**: 3096-3109.

Hansen J.P., McDonald I.R. and Pollock E.L. 1975. Statistical Mechanics of Dense Ionized Matter. III. Dynamical Properties of Classical One-component Plasma. *Phys. Rev. A* **21**: 1025-1039.

Jastrow R. 1955. Many-Body Problem with Strong Forces. *Phys. Rev.* **98**: 1479-1484.

Kalos M.H., Levesque D. and Verlet, L. 1974. Helium at Zero Temperature with Hard Sphere and Other Forces. *Phys. Rev. A* **9**: 2178-2195.

Lebowitz J., Percus J.K. and Verlet L. 1967. Ensemble Dependence of Fluctuations with Application to Machine Computations. *Phys. Rev.* **153**: 250-254.

Levesque D., Tu Khiet, Schiff D. and Verlet L. 1965. On the Ground State of Liquid and Solid He^4 at Zero Temperature. *Preprint* (unpublished).

Levesque D. and Ashurst W. 1974. Long Time Behavior of the Velocity Autocorrelation Function for a Fluid of Soft Repulsive Particles. *Phys. Rev. Lett.* **33**: 277-280.

McDonald I.R. and Singer K. 1967. Calculation of thermodynamic properties of liquid argon from Lennard-Jones parameters by a Monte Carlo method. *Disc. Faraday Soc* **43**: 40-49.

McMillan W.E. 1965. Ground State of Liquid He^4. *Phys. Rev. A* **138**: 442-452.

Mareschal M. 2018. Early Years of Computational Statistical Mechanics. *Eur. Phys. J. H.* **43**: 293-302.

Metropolis N., Rosenbluth A.W., Rosenbluth M.N., Teller A.H. and Teller E. 1953. Equation of State Calculations by Fast Computing Machines. *J. Chem. Phys.* **23**: 1087-1093.

Newton I. 1883, *Philosophiae naturalis principia mathematica.* Glasguae, Impensis T.T et J. Tegg, Londini. (http://books.google.com).

Onsager L. 1944. Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition. *Phys. Rev.* **65**: 117-149.

Ornstein L.S. and Zernike F. 1914. Accidental deviations of density and opalescence at the critical point of a single substance. *Royal Netherlands Academy of Arts and Sciences Proceedings* **17**: 793-806.

Percus J.K. and Yevick G.J. 1958. Analysis of Classical Statistical Mechanics by Means of Collective Coordinates. *Phys. Rev.* **110**: 1-13.

Principia Translation. 1934, *Newton's Principia Motte's translation 1729* revised by Florian Cajori, University of California Press, Berkeley, Los Angeles, London, p. 40-41 :
« For suppose the time to be divided into equal parts, and in the first part of that time let the body by its innate force describe the right line AB. In the second part of that time, the same would (by Law 1), if not hindered, proceed directly to c, along the line Bc equal to AB; so that by the radii AS, BS, cS, drawn to the centre, the equal areas ASB, BSc, would be described. But when the body is arrived at B, suppose that a centripetal force acts at once with a great impulse, and, turning aside the body from the right line Bc, compels it afterwards to continue its motion along the right line BC. Draw cC parallel to BS meeting BC in C; and at the end of the second part of the time, the body (by Cor. 1 of the Laws) will be found in C, ... »

Rahman A. 1964. Correlations in the Motion of Atoms in Liquid Argon. *Phys. Rev. A* **136**: 405-409.

Rosenbluth M.N. and Rosenbluth A.W. 1955. Monte Carlo Calculation of the Average Extension of Molecular Chains. *J. Chem. Phys.* **23**: 356-360.

Stauffer D. 1985. *Introduction to Percolation Theory.* Taylor and Francis, London.

Schiff D. and Verlet L. 1967. Ground State of Liquid Helium-4 and Helium-3. *Phys. Rev.* **160**: 208-219.

Schiff D. 1969. Computer "Experiments" on Liquid Metals. *Phys. Rev.* **186**: 151-160.

Thiele E. J. 1963. Equation of State for Hard Spheres. *J. Chem. Phys.* **39**: 474-479.

Verlet L. 1960. On the theory of classical fluids. *Il Nuovo Cimento* **18**: 77-101.
Verlet L. and Levesque D. 1962. On the theory of classical fluids II. *Physica* **28**: 1124-1142.
Verlet L. 1964. On the theory of classical fluids-III. *Physica* **30**: 95-104.
Verlet L. 1965. On the theory of classical fluids-IV. *Physica* **31**: 959-966.
Verlet L. 1967. Computer "Experiments" on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules. *Phys. Rev.* **159**: 98-104.
Verlet L. and Schiff D. 1974. Tribune libre : Faut-il continuer la recherche scientifique ? *La Recherche* **nov. 1974**: 924.
Verlet L. 1993. *La Malle de Newton*, Bibliothèque des Sciences Humaines, Gallimard, Paris.
Verlet L. 2007. *Chimères et Paradoxes*, Les Éditions du Cerf, Paris.
Vieillard-Baron J. 1972. Phase Transitions of the Classical Hard-Ellipse System. *J. Chem. Phys.* **56**: 4729-4744.
Wertheim M.S. 1963. Exact Solution of the Percus-Yevick Integral Equation for Hard Spheres. *Phys. Rev. Lett.* **10**: 321-323.
Wood W.W. and Parker F.R. 1957a. Monte Carlo Equation of State of Molecules Interacting with the Lennard-Jones Potential. I. A Supercritical Isotherm at about Twice the Critical Temperature. *J. Chem. Phys.* **27**: 720-734.
Wood W.W. and Jacobson J.D. 1957b. Preliminary Results from a Recalculation of the Monte Carlo Equation of State of Hard Spheres. *J. Chem. Phys.* **27**: 1207-1208.