# Computer simulation, statistics, and truth A conversation with the author of 'Chimères et paradoxes' (2007)

Werner Krauth Laboratoire de Physique, Ecole normale supérieure, Paris, France

22 January 2020 Colloquium in memory of Loup Verlet Ecole Normale Supérieure, Paris (France)

E. P. Bernard, W. Krauth, D. B. Wilson, PRE (2009)
E. P. Bernard, W. Krauth, PRL (2011)
M. Michel, S. C. Kapfer, W. Krauth, JCP (2014)
M. F. Faulkner, L. Qin, A. C. Maggs, W. Krauth, JCP (2018)

Work supported by A. v. Humboldt Foundation



### L. Verlet: 'Chimères et paradoxes'





#### L. Verlet on Models

## Métaphore, modèle et objet-chimère.

Comme l'objet transitionnel, la métaphore unit deux registres disparates, elle fore un passage de l'un à l'autre, elle se présente comme une figure paradoxale

#### L. Verlet on Models

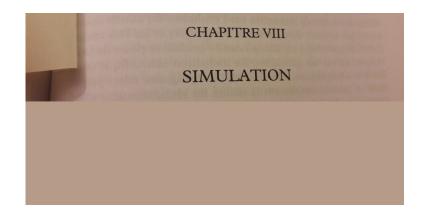
### Métaphore, modèle et objet-chimère.

Comme l'objet transitionnel, la métaphore unit deux registres disparates, elle fore un passage de l'un à l'autre, elle se présente comme une figure paradoxale

(et l'objet-chimère), le modèle est maintenu en tension entre deux pôles opposés : mitation, qui vise à une reproduction

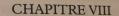
aussi fidèle que possible de la réalité perçue, et la création d'une représentation qui, tout en ressemblant à l'original, se présente clairement comme une fiction caricaturale destinée à faire ressortir des traits auparavant invisibles. Laissant à plus tard le pôle de l'imitation, qui englobe les modèles par lesquels les processus naturels sont « simulés » à l'aide des ordinateurs extrêmement puissants dont nous disposons aujourd'hui, je m'attacherai maintenant au pôle de la création : là, les modèles cherchent à révéler un ordre idéalement simple resté jusque-là

### L. Verlet on Simulation





### L. Verlet on Simulation

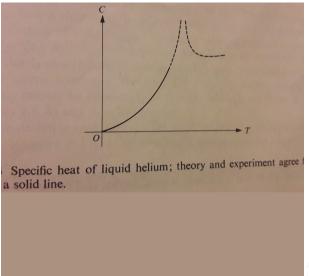


#### SIMULATION

Comme la photographie dans le domaine de l'art, la simulation se présente sous un statut hybride. Elle peut être vue comme une imitation de la réalité observée ou bien comme une création dépassant les apparences immédiates. Elle est tendue entre deux pôles – imitation et création –, qui sont précisément ceux entre lesquels vacillent le *modèle*, comme nous l'avons vu

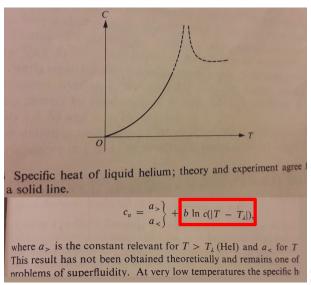


### R. P. Feynman 'Statistical Mechanics' (1961) 1/2





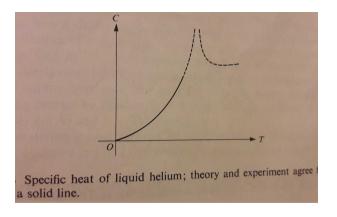
### R. P. Feynman 'Statistical Mechanics' (1961) 2/2







### $\lambda$ transition (renormalization-group predictions)



$$C \sim |T - T_c|^{-\alpha}$$
 where  $\alpha = \frac{2\Delta_s - 3}{3 - \Delta_c}$ 

•  $O(2) \rightarrow Z_2$  symmetry breaking.



### $\lambda$ transition (observed reality)



Image above: STS-52 Crew photo with Commander James D. Wetherbee, Pilot Michael A. Baker, Mission Specialists Charles L. Veach, William M. Shepherd, Tamara E. Jernigan and Payload Specialist Steven A. MacLean. Image Credit:



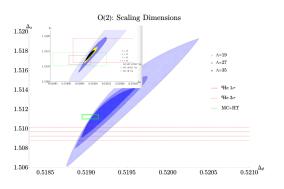
The primary mission objectives were the deployment of the Laser Geodynamic Satellite II (LAGEOS-II) and operation of the U.S. Microgravity Payload-1 (USMP-1). LAGEOS-II, a joint effort between NASA and the Italian Space Agency (ASI), was deployed on day two and boosted into an initial elliptical orbit by ASI's Italian Research Interim Stage (IRIS). The spacecraft's apogee kick motor later circularized LAGEOS orbit at its operational altitude of 3,666 miles. The USMP-1, which was activated on day one, included three experiments mounted on two congected Mission Peculiar Equipment Support Structures (MPESS) mounted

in the orbiter's cargo bay. USMP-1 experiments were Lambda Point Experiment Materiel Pour L'Etude Des Phenomenes

- Columbia Space Shuttle mission STS-52 (1992).
- Experiment by Lipa et al. (1996), (2003).
- $\alpha = 0.0127(3)$ .



### $\lambda$ transition (theory + observed reality)



- Campostrini et al. (2005): 3D XY model, Cluster MC + HTE.
- Xu et al. (2019): 3D XY model, worm algorithm.
- ullet Hasenbusch (2019): (N + 1)-state clock model, Cluster MC
- ullet Chester et al. (2019): Conformal bootstrap for  $O(2) o Z_2$

### Xu, Sun, Lv, Deng (2019)

Model	Ref.	Method	Year	$T_c$ or $(t/U)_c$
XY	[15]	MC MC MC MC MC (GPU) MC (GPU) MC (GPU)	1993	2.201 67(10)
	[32]	MC	1996	2.201 843(19)
	[33]	MC	2002	2.201 833(19)
	[31]		2005	2.201 840 5(48)
	[13]		2012	2.201 831 2(6)
	[13]	MC (GPU)	2012	2.201 852(1)
	[14]	MC (GPU)	2014	2.201 836(6)
	this work	MC	2019	2.201 844 1(5)

- Transition temperature of the 3D XY model.
- Non-universal model input required for computation of universal  $\alpha$ .



### What's the required samples size n?

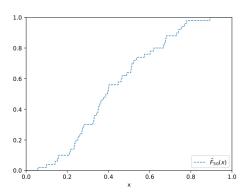


'Non-chimeric' computations do not require  $n \to \infty$  limit.





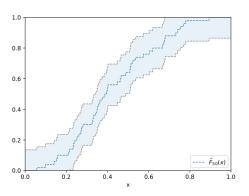
### Dvoretzky-Kieffer-Wolfowitz inequality (1956) 1/3



- Empirical CDF  $\hat{F}$ , no hypothesis on (atomic) CDF F.
- (Cumulative distribution function).



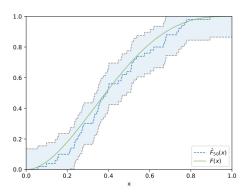
### Dvoretzky-Kieffer-Wolfowitz inequality (1956) 2/3



- Empirical CDF  $\hat{F}$ , iid samples.
- 'Corridor', no hypothesis beyond iid.



### Dvoretzky-Kieffer-Wolfowitz inequality (1956) 3/3



- $P[\sup_{x} |F_n(x) F(x)| > \epsilon] \le 2 \exp(-2n\epsilon^2)$ .
- Tight constraint: Massart (1990), figure by Botao Li.



### What's the required run time t?



Non-chimeric computations do not require  $t \to \infty$  limit.



### Perfect Markov-chain sampling

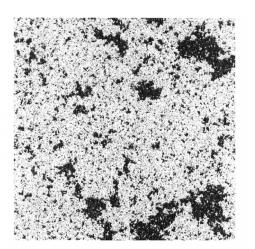
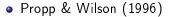


Fig. 1. An equilibrated Ising state at the critical temperature on a  $4200 \times 4200$  toroidal grid.





### Liquids and computations on liquids





### Metropolis et al (1953) (1/2)

URNAL OF CHEMICAL PHYSICS

VOLUME 21. NUMBER 6

JUN

#### Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,

Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD Teller,\* Department of Physics, University of Chicago, Chicago, Illinois (Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.



### Metropolis et al (1953) (2/2)

1092 METROPOLIS, ROSENBLUTH, ROSENBLUTH, TELLER, AND TELLER



distinguished by primes. For example,  $A_{33}$  is given schematically by the diagram



and mathematically as follows: if we define  $f(r_{ij})$  by

$$f(r_{ij}) = 1 \quad \text{if} \quad r_{ij} < d,$$
  
$$f(r_{ij}) = 0 \quad \text{if} \quad r_{ij} > d,$$

then

$$A_{3,3} = \frac{1}{\pi^2 d^4} \int \cdots \int dx_1 dx_2 dx_3 dy_1 dy_2 dy_3 (f_{12} f_{23} f_{31}).$$

The schematics for the remaining integrals are indicated in Fig. 6.

The coefficients  $A_{3,3}$ ,  $A_{4,4}$ , and  $A_{4,5}$  were calculated

were put down at random, subject to  $f_{12}=f_{22}=f_{24}=f_{15}=1$ . The number of trials for which  $f_{45}=1$ , divided by the total number of trials, is just  $A_{5.5}$ .

The data on  $A_{4,6}$  is quite reliable. We obtained

#### VI. CONCLUSION

The method of Monte Carlo integrations over configuration space seems to be a feasible approach to statistical mechanical problems which are as yet not analytically soluble. At least for a single-phase system a sample of several hundred particles seems sufficient. In the case of two-dimensional rigid spheres, runs made with 50 particles and with 224 particles agreed within statistical error. For a computing time of a few hours with presently available electronic computers, it seems possible to obtain the pressure for a given volume and temperature to an accuracy of a few percent.

In the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for  $A/A_0 < 1$ -Sandawith an investment in the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for  $A/A_0 < 1$ -Sandawith an investment are in the case of two-dimensional rigid spheres our results are in agreement and the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for  $A/A_0 < 1$ -Sandawith an investment and  $A/A_0 < 1$ -Sandawith and  $A/A_0$ 

for  $A/A_0 \ge 2.5$ . There is no indication of a phase

transition.



### Alder–Wainwright (1962)

PHYSICAL REVIEW

VOLUME 127, NUMBER 2

JULY 15, 1962

#### Phase Transition in Elastic Disks\*

B. J. Alder and T. E. Wainwright
University of California, Laurence Radiation Laboratory, Livermore, California
(Received October 30, 1961)

The study of a two-dimensional system consisting of 870 hard-disk articles in the phase-transition region has shown that the isotherm has a wan der Waals-like loop. The insity change across the transition is about 4% and the corresponding entropy change is small.

A STUDY has been made of a two-dimensional system crossisting of 870 hard-disk particles. Simultaneous motions of the particles have been calcuated by means of an electronic computer as described previously. The disks were again placed in a periodically repeated rectangular array. The computer program

interchanges it was not possible to average the two branches.

Two-dimensional systems were then studied, since the number of particles required to form clusters of particles of one phase of any given diameter is less than in three dimensions. Thus, an 870 hard-disk system is



### Kosterlitz-Thouless (1973)

# Ordering, metastability and phase transitions in two-dimensional systems

J M Kosterlitz and D J Thouless

Department of Mathematical Physics, University of Birmingham, Birmingham B15 2TT, UK

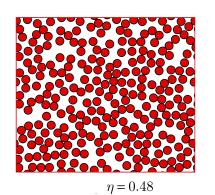
Received 13 November 1972

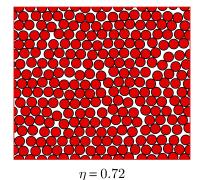
#### 1. Introduction

Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the diffraction pattern formed by the system are broad instead of sharp. The absence of long-range order of this simple form has been shown by Mermin (1968) using rigorous inequalities. Similar arguments can be used to show that there is no spontaneous magnetization in a two-dimensional magnet with spins with more than one degree of freedom (Mermin and Wagner 1966) and that the expectation value of the superfluid order parameter in a two-dimensional Bose fluid is zero (Hohenberg 1967).

On the other hand there is inconclusive evidence from the numerical work on a two-dimensional system of hard discs by Alder and Wainwright (1962) of a phase transition between a gaseous and solid state. Stanley and Kaplan (1966) found that high-temperature series expansions for two-dimensional spin models indicated a phase

### Possible phases in two dimensions

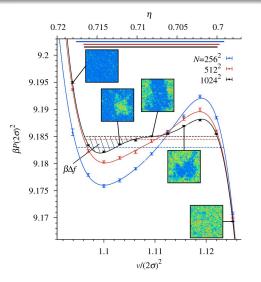




Phase	positional order	orientational order
solid	algebraic	long-range
hexatic	short-range	algebraic
liquid	short-range	short-range



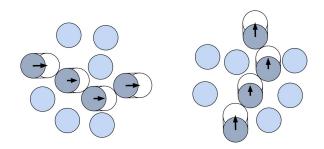
### Equilibrium equation of state



• 1st-order liquid-hexatic (Bernard & Krauth, PRL (2011)).



### Irreversible Markov chains in equilibrium statistical physics



- Bernard, Krauth, Wilson (2009).
- Infinitesimal moves: consensus.
- Michel, Kapfer, Krauth (2014) (smooth potentials).



### Factorized Metropolis algorithm

Metropolis algorithm

$$ho^{\mathsf{Met}}(a o b) = \mathsf{min}\left[1, \prod_{i < j} \mathsf{exp}\left(-eta \Delta \mathit{U}_{i,j}
ight)
ight]$$

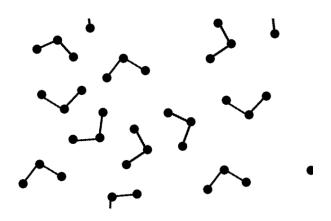
Factorized Metropolis algorithm (Michel, Kapfer, Krauth 2014)

$$p^{\mathsf{Fact.}}(a o b) = \prod_{i < i} \min \left[ 1, \exp \left( - \beta \Delta U_{i,j} \right) \right].$$

$$X^{\mathsf{Fact}}(a \to b) = X_{1,2} \land X_{1,3} \land \cdots \land X_{N-1,N}$$



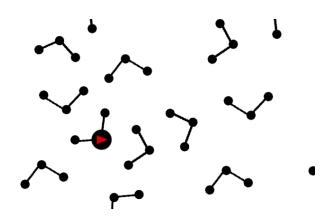
### All-Atom Coulomb problem (1/5)



• 3D water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).



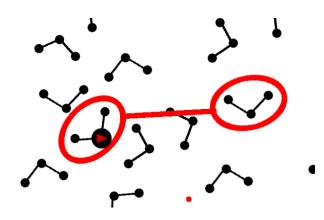
### All-Atom Coulomb problem (2/5)



- 3D water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).
- Factors and types.



### All-Atom Coulomb problem (3/5)

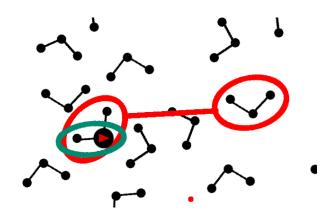


• Factor  $M = (I_M, T_M)$ :  $|I_M| = 6$ , two molecules.  $T_M =$  'Coulomb'.





### All-Atom Coulomb problem (4/5)

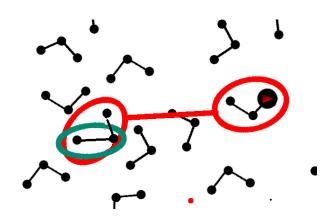


 Water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).





### All-Atom Coulomb problem (5/5)

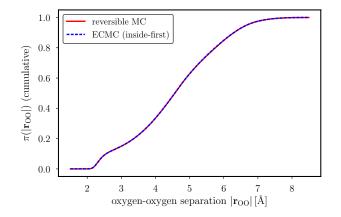


- Complexity  $\mathcal{O}(1)$  per 'lifting' move.
- This is the cell-veto algorithm (Kapfer, Krauth (2016)).
- Thinning, Walker (1977).



#### ECMC for all-atom water simulations

- ECMC: Event-driven, approximation-free, canonical.
- ECMC: Potential U not evaluated to sample  $\exp(-\beta U)$ .



- See: Faulkner, Qin, Maggs, Krauth (2018).
- See: Hoellmer, Qin, Faulkner, Maggs, Krauth (2020).



### Conclusions

- Golden age of physics, and of statistics.
- Universality of models.
- Computation: road to knowledge.
- Loup Verlet: a constant inspiration.



