Genetic Algorithms and Critical Phenomena

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Abstract

Genetic algorithms based on natural selection and minimal fluctuations have been applied to model physical and biological systems. Critical exponents have been extracted via computational simulations of nucleation for colossal magnetoresistance, heavy ions liquid-gas phase transitions and HIV to AIDS transition.

1 Introduction

We have developed genetic algorithms to study the evolution of several finite physical systems starting from an initial state, until an absorbing state is reached. Phase transition is identified with fragment build up and the critical multiplicity is the one providing the best $\chi^2$ test.

Since Fisher Liquid Droplet Model as well as Random percolation show a power law near the critical point, we may speculate whether both belong to the same universality class. In both cases finite size and geometry effects are also anticipated. Even when these systems have a different physical nature, the fact that correlations are increased close to the critical point leads us to question whether these belong to the same universality class. This is extended to the VIH to AIDS transition, which can be modeled as a nucleation process whose critical exponents were hereby extracted.

The behavior close to the critical point is characterized by a loose of time and space scales, which promotes the similarity among all the critical phenomena, independently of their specifics. In the case of the transient and finite systems, the most important scales are system size and reaction duration, though critical phenomena will not always occur. Hence, it is important to prove the feasibility of critical behavior in these finite dynamical systems.

First neighbor particle correlations are not present in gases though liquids exhibit strong first neighbor two body correlations. Hence, correlations grow close to the critical point, including all particles of the

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system. Therefore, the influence of geometry should be considered as well as class universality of different physical systems should be questioned [1].

Even when power laws have been observed in distinct physical systems, such as seismic distributions, fractal coastlines, weather records and DNA statistics [2], it is well known that log-log plots are able to depict spurious linear relations. This would result from a self-organized criticality (SOC), where non-equilibrium systems should move slowly through an instability with a global and local relaxing mechanism. Also, these anomalous power laws can be related to codimension one critical points, where a critical behavior is reached after a temperature fluctuation even when this could not arise from a natural evolution of the system [3]. Therefore, it is important to perform simulations of theoretical models in order to prove the feasibility of the critical behavior associated with these power laws.

Cohen et. al. extracted of critical exponents scale-free networks, where a power law holds: \( P(k) = ck^{-\lambda}, k \geq m \), with \( P(k) \) equal to the probability of a node being connected to exactly \( k \) nodes [4]. Grassberger obtained percolation thresholds for simple hypercubic lattices whose dimension goes from 4 to 13, finding anomalous scaling when \( d \geq 7 \): \( M(t) = M_\infty - \frac{\text{const.}}{t^\alpha} \), where \( M(t) \) is the number of wetted sites at step \( t \) and the scale correction is in agreement with the following power law: \( M_\infty - 1 \sim (d - 6)^{-\alpha} \) [5].

Fortunato and Satz studied the explicit symmetry breakup for spin models, finding that in the case of a second order phase transition with a small field, the percolation thresholds line lies parallel to the susceptibility peak line (pseudo critical line). And the first order phase transition line is a percolation transition line, though the critical exponents are not equal to those belonging either to the random percolation model or the Ising model [6]. This leads to consider a new cluster definition that takes on account the magnetic field intensity, which could be used to study QCD deconfinement with dynamical quarks [7].

Coniglio postulated that above the critical dimension, the number of percolation clusters is infinite and hyperscaling relation no longer holds : \( 2 - \alpha = \nu d \) [8]. This was proven by Andronico et. al. for the case of random percolation, though this does not hold for the Ising model due to distinct behaviors below and above the critical temperature [9].

The manuscript is organized in the following way. In the second section Fisher nucleation theory is described, showing how to extract the critical exponents close to the critical multiplicity. In the third section some reasons are given to expect this power law for a percolation system and the expected values for some percolation systems are shown. In section IV a genetic algorithm for HIV to AIDS transition is described, and its critical exponent is extracted. In section V a genetic algorithm is used to compute the critical exponent of the Colossal Magnetic Resistance. Section VI describes the Molecular Dynamics simulation employed to compute the critical exponent for the liquid-gas phase transition in Heavy Ions as well as the simulated annealing algorithm used to detect clusters. In section VII some conclusions are established from these results.
2 Fisher Liquid Droplet Model

According to fluctuation theory [10], the probability to obtain a liquid droplet of radius \( r \) and \( A \) nucleons in a vapor at temperature \( T \) is given by [11]:

\[
P_r(A) = Y_0 A^{-\tau} e^{-\left((\mu_l - \mu_g)A + 4\pi r_0^2 \sigma(T)A^{2/3}\right)/T},
\]

where \( \Delta G \) is the change due to the phase transition in Gibbs Free energy. This includes surface, curvature and bulk energy terms. In the coexistence region, nevertheless, \( (\mu_l - \mu_g) = 0 \), and:

\[
P_r(A) = Y_0 A^{-\tau} \exp[-4\pi r_0^2 \sigma(T)A^{2/3}/T]
\]

Finally, in the critical point: \( (\mu_l - \mu_g) = 0 \), but as the liquid and vapor are indistinguishable at this point, surface energy is null: \( \sigma(T_c) = 0 \), hence the distribution is

\[
P_r(A) = Y_0 A^{-\tau},
\]

namely a pure power law, and as such, scale free. The exponent \( \tau \) appearing in the droplet size distribution (1), is known as the critical exponent since it is a dimensionless constant with a common value for different systems.

Fisher Liquid Droplet Model (FDM) for nucleation [12] refines the probability (1) to obtain a critical mass distribution normalized to the size of the system:

\[
n_A = q_o A^{-\tau}
\]

with a proportionality constant \( q_o \) that can be obtained using the first moment, \( M_1 = \sum_A n_A A \) of the normalized mass distribution, (i.e. \( M_1 = 1 \)). Therefore \( q_o \) can be obtained with the following equation: \( q_o = 1/\sum_A A^{(1-\tau)} \). In order to select critical events, critical multiplicity is identified as the one providing the optimal \( \chi^2 \) fit [13].

Supposing scaling for the fragment size distributions, close to the critical point:

\[
M_k \sim \left| T - T_c \right|^{(-1-k+\tau)/\sigma}
\]

where: \( 2 < \tau < 3 \). Critical exponents are given by the following expressions [14]:

\[
M_2 \sim |\epsilon|^{-\gamma}
\]

\[
A_{\text{max}} \sim |\epsilon|^\beta
\]

when \( m = m_c \).

3 Percolation critical exponent

A great variety of percolation methods have been used ever since Flory introduced percolation in the context of polymer gellation [15]. For many spin models, there exists a mapping of the equivalent graphic representation of a percolation transition corresponding to a spin model phase transition [16].
Harreis and Bauer introduced a method to deal with $N$ component percolation, finding new first order phase transitions and new empirical formulas for the percolation threshold as a function of component concentration [17]. Bauer introduced percolation in the study of fragmentation [18, 19], vid. Stauffer [20] for more details.

A percolation cluster has activated bonds going from one side of the lattice to the opposite side. For infinite systems, there is a well defined “critical probability” $p_c$, above which the probability to find a percolation cluster is equal to 1, meanwhile below $p_c$ this probability is equal to 0. For finite lattices, this transition is soft, i.e. the probability to find a percolation cluster is not equal to 0 for any probability. Mader et.al. have shown reducibility and thermal scaling properties in the Ising model, obtaining a value of $\tau = 2.39$ [21]. Chayes et.al. have shown a finite cluster scaling critical exponent $\tau - 2 = 1/2$ and an infinite cluster scaling critical exponent $\tau - 2 = 1/2$ [22]. In the percolation model the weight of a given configuration $C$ of $n$ links is given by:

$$W(C) = p^n (1-p)^{N-n}$$

where $N$ is the number of vertices in the lattice. Close to the percolation threshold, the critical behavior is characterized by the following critical exponents:

$$P_\infty = 1 - \sum s n(s, p) \sim |p - p_c|^\beta$$

and:

$$S(P) = \sum s^2 n(s, p) \sim |p - p_c|^\gamma$$

Cluster distribution satisfies the following scaling relation:

$$n(s, p) = s^{-\tau} f((p - p_c)s^\sigma)$$

hence a power law is expected close to the critical point:

$$n(s, p) = s^{-\tau} f(0)$$

Starting from these relations, the following equations can be obtained:

$$\tau = 2 + \frac{\beta}{\beta + \gamma}$$

and:

$$\sigma = \frac{1}{\beta + \gamma}$$

In 3D, the best estimation is $\tau = 2.18$ and $\sigma = 0.45$ [23]

Bauer y Golinelli have obtained a second order phase transition when $\alpha = \epsilon = 2.718...$ in the percolation of random graphs whose connectivity is $\alpha$ and where the leaves and their neighbors are iteratively removed. In that study, a new power law was found for $N_C$, the number of vertices in the core tree: $N_C \sim N^{\omega}$, where $N$ is the number of vertices of the original graph [24]. Power laws have been found in statistical distributions of Hamming distances for random threshold networks and random binary lattices with scale-free distributions whose interior degree $\sim k_m^\alpha$ [25].

Kamp and Bornholdt have studied percolation transition in a directed graph, with activating and deactivating bonds, and extracted power law
critical exponents for the number of avalanches as a function of active
sites, as well as a plot of the fraction of activating bonds versus system
size [26].

Bornholdt and Rohlf have studied a symmetrically connected threshold
lattice whose topology is changed with a local rule, obtaining a power law
in the plot of mean connectivity versus system size [27].

4 HIV Cellular Automaton

Ebel et. al. found power laws for the avalanche size distribution given
by the number of mutations required to establish an equilibrium in evolution-
ary games with Nash equilibriums perturbed by mutant events [28].

When mutation rates are close to a substitution for each genome of
each generation, a virus population forms a highly diversified cloud of
mutants [29]. Since sequence space is quite large, even for a population size
of the order of $10^{12}$ there is a constant flux of brand new mutants. With
some probability these mutants will fixate, where fixation is understood
as the moment in which a mutant comes out to be the ancestor of a new
quasi-species that fully replaces the old one.

In the quasi-species configuration, on the other side, most of the pro-
genies of a mutant suffers subsequent mutations and also its progenies.
Therefore, a new species adaptation is not given by the adaptation of the
first mutant, but by the the mean adaptation of the eventually formed
mutant cloud.

Wilke has shown, using a multibranching processes model, that fixa-
tion depends on the global rate of growth of the quasi-species obtained due
to an infection [30]. Asexual organisms genomic mutation rates, such as
bacteria and ADN, have been observed in the range of $2 \times 10^{-3} \sim 4 \times 10^{-3}$,
hence a few in a thousand mutate [31]. Smaller genomic mutation rates
have not been observed since adaptability to a changing environment is re-
quired for a species [32]. Wilke has proved, based on quasi-species model,
that in the case of low mutation rates, population could benefit on envi-
ronment fluctuations [33].

4.1 HIV Cellular Automaton

Population evolution has been modeled using Kamp cellular automaton,
reproducing HIV to AIDS transition, though in this study we focus on
the nucleation of infected cells as well as the seldom observed incapability
of HIV to evolve into AIDS [34]. According to Kamp, in an infection,
viral genomes are diversified due to mutation and selective pressure of
the immune system. This coevolutionary dynamics can be modeled in
sequence space. Viral genomes can be represented by chains of length
$n$, built up from an alphabet of length $\lambda$ and their diversification can be
described as a dispersion in sequence space. Analogously, we assign a
sequence to the immune receptor corresponding to the viral strain. Any
chain in sequence space is supposed to represent a viral epitome, as well
as its complementary immune receptor.
Therefore, each sequence is characterized by a viral and immune state variable. A site in sequence space is susceptible if it can host a virus. It is called infected if the system has a virus with an epitome motif represented by the chain of the site. If a viral sequence finds an immune response it is removed and the system is immunized against it. In this case, and in the case where a site is unreachable for virus, it is called recovered (or removed).

Since viral and immune entities replication is affected by copy fidelity: $q_{vs} < 1$ and $q_is < 1$, system shows viral and immune dispersion in sequence space. Introducing some viral strains in a system originally free of them, a dynamic evolution follows from the cellular automaton approximation after the following iteration steps [34]:

Kamp automaton proceeds in the following way. A random site is chosen and a) if the site represents an immune receptor, a randomly chosen bit is mutated with probability $(1-q_{is})$, or, b) if a new immune strain is generated and the mutant coincides with a site, the site is considered as a recovered site. If the site is infected, a bit is randomly changed with probability $(1-q_{vs})$, or, if a new immune strain is generated and the mutant coincides with a susceptible site, the site is considered as infected.

4.2 Results

A critical exponent was extracted with a value of $\tau = 2.32$ for the power law of infected cells of HIV to AIDS transition, simulated with a genetic algorithm that evolves populations with a cellular automaton (Fig. 1).

Besides, infected site ratios were obtained as a function of genetic variability of both infected sites $q_{vs}$ and healthy sites $q_{is}$. As can be appreciated in (Fig. 2), two regions of low infected sites ratios are formed, which ensures an immune response, for low and high values of genetic variability. This explains the observed capability of some immune systems to resist viral infections, notwithstanding high genetic mutation rates would lead to the opposite scenario.

5 Colossal Magnetoresistance

Lübeck has computed the critical exponents and the fluctuations of the order parameter, for the case of a conservative lattice, finding a maximum critical dimension for this gas equal to 4 [35]. Mari et al. have performed corrections for the finite size of the system, in the case of the Binder parameter of the 3D binomial Ising spin glass [36]. Janssen et al. have shown that for a vector magnetic system of order N, when the temperature is much greater than the critical temperature, and the system is suddenly compressed until the critical state, a dynamical scaling is installed in the early evolution of the system [37].

Ying et al. found a relation between the binding randomness and the critical universality for the Potts random binding ferromagnet with a ternary distribution of compressed disorders in triangular lattices [38].

Simões et al. studied the early evolution dynamics for the two dimensional Ising model with three spin interactions in a direction, taking on
account the symmetry of the Hamiltonian and the boundary conditions when computing magnetization. They obtained the same critical exponents of the four states Potts model [39].

Ying et al. studied the early dynamics and critical universality for the Potts model with q=2 and q=3 in triangular two dimensional lattices, obtaining critical exponents equal to those of the corresponding two dimensional square lattice, concluding that they belong to the same universality class [40].

Acharyya et al. computed the critical temperature of the metamagnet FeBr$_2$, using the anisotropic classical Heisenberg model, in a tetragonal lattice, finding that for high temperatures there is a first order phase transition between a paramagnetic phase and a flipped spin tilted phase. And for low temperatures, the phase transition is discontinuous and from a flipped spin tilted phase up to a longitudinal ferromagnetic phase [41].

In this study three dimensional configurations were generated, randomly assigning three spin values $S = -1, 0, 1$, with the following Hamiltonian:

$$H = -J \sum_{i,j} S_i S_j - H \sum_i S_i.$$  \hspace{1cm} (13)

A site is randomly chosen and its value is changed with the following probability:

$$p = \frac{e^{-\Delta H/T}}{1 + e^{-\Delta H/T}}.$$  \hspace{1cm} (14)

5.1 Results

The extracted critical exponent for the colossal magnetoresistance is 2.39 (Fig. 3). Besides, we have computed a critical exponent $\beta = 0.38$, suggesting that it belongs to the universality class of Heavy Ion Collisions, as shown in Table 1. The obtained value of $\beta$ is close to the one reported by Kudzia et al. in fragmentation experiments on Au emulsions [42]. The spontaneous susceptibility plot indicates a critical temperature close to 4.5 K (Fig. 4).

6 Simulations of Heavy Ion Collisions

Among the signals used to search for nucleation in nuclear systems, the presence of a peak in the specific heat has been used as a phase transition signature for periodical systems [43].

Another signature explored is the controversial power law of the fragment distribution, close to the critical point of a liquid-gas phase transition [44]. In the energy range of relativistic Heavy Ion Collisions, a phase transition has been associated with the onset of shock wave front instabilities [45].

In Heavy Ion Collisions, a phase transition is expected to turn into a second order phase transition in the critical point of the phase diagram (Fig. 5). Experimental measurements of Au+Au collisions performed at GSI, were used to build a plot of temperature versus excitation, providing
evidence of phase coexistence, in agreement with predictions of statistical multifragmentation models excluding volume [46]. Other experiments performed in Bevalac extracted critical exponents and studied the dependency of both the second moment of charge distribution and the biggest fragment size on charged particles multiplicity. These data were consistent with a second order phase transition predicted by the percolation model [47].

6.1 Molecular Dynamics

A Molecular Dynamics realistic model, nicknamed “LATINO Model” [48, 49] has been used. This three dimensional model uses a Pandharipande binary potential that reproduces the energy and empirical density of nuclear matter, as well as realistic effective scattering cross sections. Nuclei used hereby were spherical droplets with the desired number of protons and neutrons, produced as ground states using Molecular Dynamics. Once a spherical nuclear system is randomly created at a high temperature, it is cooled until it reaches a self-contained state. At this moment, the confining potential is removed and the system is cooled until it reaches a reasonable binding energy. Collision is simulated boosting one of the nuclei against the other and integrating the coupled equations of motion using a Verlet algorithm, ensuring an energy conservation better than a 0.01% (Fig. 6).

6.2 Fragment Recognition

In order to transform particle information provided by Molecular Dynamics in terms of fragment information, an Early Cluster Recognition Algorithm is needed, such as the algorithm that finds the most bound partition of the system [50], i.e. the set of clusters \( \{ C_i \} \) for which the sum of internal energies of the fragments attains a minimum value:

\[
\{ C_i \} = \text{argmin}_{\{ C_i \}} [E_{\{ C_i \}} = \sum_i E_{C_i}^{\text{int}}]
\]

\[
E_{C_i}^{\text{int}} = \sum_i \left[ \sum_{j \in C_i} K_{j, \text{cm}}^\text{cm} + \sum_{j,k \in C_i, j \leq k} V_{j,k} \right]
\]

where the first sum is on partition clusters, \( K_{j, \text{cm}}^\text{cm} \) is the kinetic energy of particle \( j \) measured in the center of mass of the cluster containing particle \( j \), and \( V_{j,k} \) is the internucleonic potential. The algorithm that uses “simulated annealing” to find the most bound partition is known as “Early Cluster Recognition Algorithm” (ECRA) and has been extensively used in several fragmentation studies [51, 50, 52], helping to discover that excited droplets breakup at an early stage.

6.3 Results

A snapshot sequence of a typical Ni+Ni central collision at 1500 MeV (Fig. 7) is shown. Increasing the projectile energy, fragmentation region is reached where phase coexistence is found and a fragment distribution
power law appears (Fig. 8). Critical exponent has been extracted for Ni+Ni central collision with a value \( \tau = 2.18 \).

7 Conclusions

Table 1 shows the critical exponent values extracted in this study and compared with others previously reported and obtained from percolation and 2D Molecular Dynamics simulations with a Lennard-Jones potential [53]. Heavy Ion Collisions Molecular Dynamics simulations as well as genetic algorithm results for colossal magnetoresistance and HIV to AIDS transition indicate that critical nucleation occurs for small and complex systems, static as well as transient, and suggest that they belong to the same universality class.

| Nucleation Model                      | \( \tau \) Value |
|---------------------------------------|-------------------|
| HIV Cellular Automaton                | 2.32              |
| Colossal Magnetoresistance            | 2.38              |
| 3-D MD Collision Simulations          | 2.18              |
| Cubic Lattice Percolation[53]         | 2.32 ± 0.02       |
| Spherical Lattice Percolation[53]     | 2.20 ± 0.1        |
| 2-D Collision Simulations[53]         | 2.32 ± 0.02       |

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