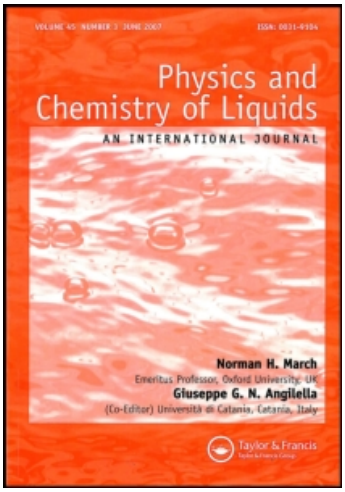

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

Numerical Experiments on Interactions and Clustering Phenomena

Jorge R. Busch[a]; David H. Kurlat[a]
[a] Facultad de Ingeniería-Paseo Colón, Buenos Aires, Argentina

To cite this Article Busch, Jorge R. and Kurlat, David H.(2000) 'Numerical Experiments on Interactions and Clustering Phenomena', Physics and Chemistry of Liquids, 38: 5, 527 — 535
To link to this Article: DOI: 10.1080/00319100008030301
URL: http://dx.doi.org/10.1080/00319100008030301

Phys. Chem. Liq., 2000, Vol. 38, pp. 527–535
Reprints available directly from the publisher
Photocopying permitted by license only

NUMERICAL EXPERIMENTS ON INTERACTIONS AND CLUSTERING PHENOMENA

JORGE R. BUSCH and DAVID H. KURLAT*

Facultad de Ingeniería-Paseo Colón 850-1063 Buenos Aires-Argentina

(Received 21 July 1999)

In this work we study, by simulation in a two dimensional lattice, the influence of diverse parameters of the interaction potential on the geometry of a system of particles. The geometry of the system is described by means of the scaling behaviour of concentration, quantified by the fractal box-counting dimension, and the configurations are sampled by means of the Metropolis algorithm. The mean concentrations of the systems studied are below and near the percolation threshold, since the main application of our study is the analysis of the scaling behaviour of conductivity in dynamic percolating systems. We show how a detailed analysis of the behaviour of concentration at different scales enlights the interplay between two correlation lengths in the system: the one due to interactions, the other due to geometrical contiguity. The description of this interplay is essential to understand the deep roots of the universality of the exponents in percolation theory, and their physical implications.

Keywords: Fractal dimension; clusters; percolation

1. INTRODUCTION

The special problem of the influence of interactions between the particles on the percolation phenomena has been addressed in [2], where it is shown to be far from trivial. The main purpose of this paper was to describe the influence of interactions on the value of the threshold ϕ_c. Following the ideas from this paper, we see that attractive interactions

*Corresponding author. Dto. de Física. e-mail: dkurlat@tron.fi.uba.ar

affect the percolation phenomena in two ways:

1. They increase the connectivity, because near particles come to be in contact.
2. They decrease connectivity, because the compactation of clusters affects the relation radius to mass.

It is rather natural to ask ourselves how these two geometrical facts affect the fractal dimension d_c of the clusters. By the universality hypothesis the exponent d_c should not be affected by the short range interactions for concentrations near the percolation threshold. On the other hand, the compaction argument seems to imply a modification on fractal dimension. Thus, we see that the invariance of these fractal dimensions under the interactions is an essential fact for the description of how they affect the geometry of the clusters. This is the main subject of our work.

We use the Metropolis algorithm [1, §4.4] to generate sample configurations of particles in a two-dimensional square lattice. The adjustable parameters for the simulations are the density of particles, the intensity of the square attractive potential and its range of attraction. Notice that the intensity of the potential is, due to Boltzmann law, numerically equivalent to the inverse temperature, thus we do not treat them as independent parameters. In this first approach, we measure the box-counting fractal dimensions d_f of the whole configurations, rather than those of the clusters, to have an insight about their sensitivity to the interactions. To estimate the box-counting fractal dimensions we use the program df2 from the public domain package "mfrac" by Jordi Mach (jordi@daphne.qf.ub.es), modified as we shall describe in the following section.

2. NUMERICAL EXPERIMENTS

As we have already mentioned, the adjustable parameters for our simulations are the density, the inverse temperature (equivalent to the intensity of the potential), and the range of the potential.

We start with a regular disposition of the particles (we assume everywhere, and this is relevant when we speak of density, that the particles are 2×2 squares) in a regular lattice 200×200, and then we

let the Metropolis algorithm perform its importance sampling of configurations. Let us call cycle a sequence formed by one movement for each particle, where the particles are moved always in the same order. Then we capture a slide of the configuration every ten cycles, and we compute its box-counting fractal dimension. Recall that this computation can be described as:

1. For each size ε from a logarithmic equispaced sequence, estimate the mean count $N(\varepsilon)$ of boxes having particles in its interior in a regular partition of size ε of the lattice.
2. The box-counting dimension is estimated by the negative of the slope of the linear regression of $\ln(N(\varepsilon))$ *versus* $\ln(\varepsilon)$, according to the model $N(\varepsilon) \propto \varepsilon^{-d_f}$.

2.1. A Small Size Effect

A general fact in this process was that dimensions increase with density. When ε is less than the mean distance between particles, in a finite random environment there is no scaling, and $N(\varepsilon)$ is asymptotically constant. The effect *via* the regression is to lower the dimension. This effect is greater for low concentrations, because then the mean distance is bigger. This small box size phenomena made our box-counting dimensions artificially sensitive to density, so we modified the ε range in df2 to exclude this effect, starting the box sizes at this mean distance.

2.2. General Clustering Effect

A second general fact in this process is that dimension decreases in the first cycles, relaxing quickly to a constant value. We explain this fact as a clustering effect of the interactions and temperature (not yet a percolation effect). Indeed, we can represent our configurations at low densities as a random assembly of boxes, each containing a small cluster or not [3, §2.3] (this is nothing but a rephrasing of the meaning of a scaling exponent d for concentration). In this representation, the side of the boxes is above the scale of the correlation length. When the side of the boxes in our box-counting algorithm is above the mean distance between these clusters, the corresponding number of boxes

scales as ε^{-2}. But when the side is below this mean distance and the mean radius of the clusters, there is a constant factor for the number of clusters, and in this scale we see roughly the behaviour ε^{-d_c}, where d_c denotes the dimension of a cluster. Thus the global regression slope is the resultant of a d_c slope for small boxes and 2 for big boxes, and we see that we can think of the resulting dimension d_f as a weighted mean of d_c and 2, let us say $d_f = \theta d_c + (1-\theta)2$. At random or with a particle regular distribution, there is no regular clustering at low density, and $\theta = 0$. But the effect on interactions and temperature promotes clustering leaving room for greater holes, increasing θ and lowering d_f. Notice that our explanation of the resultant value d_f in the regression is based on the extreme slopes, and that what we really see in our experiments is a rather slight modification in the slopes during the initial clustering process (see Figs. 1, 2).

Notice also that our explanation is somewhat analogous to our previous one on the artificial sensitivity to density: the point is that now the effect is not artificial, because in the renormalization we have

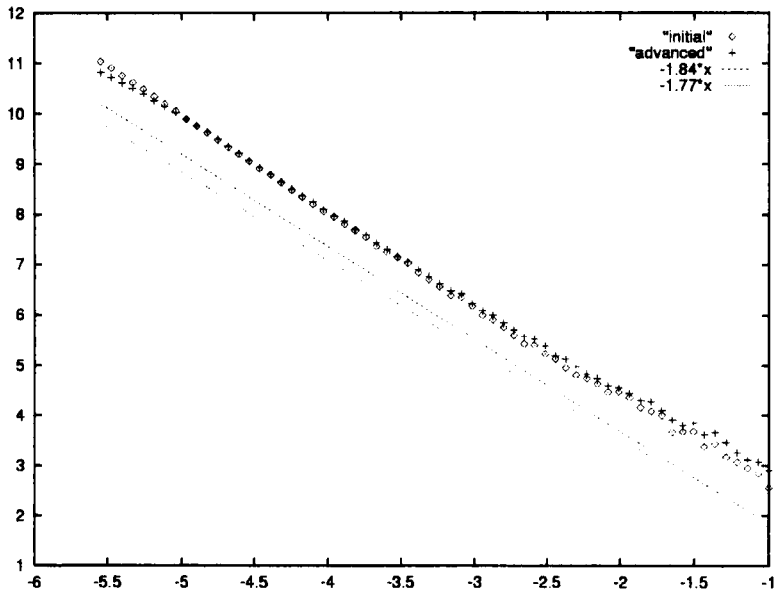

FIGURE 1 The contrast between an initial configuration (ten cycles, $d_f = 1.84$) and an advanced one (two hundred cycles, $d_f = 1.77$).

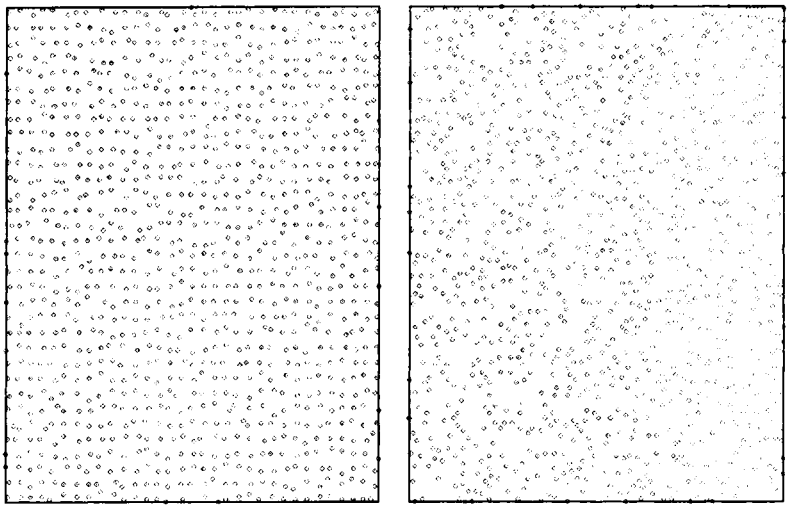

FIGURE 2 The clustering effect induced by interactions and temperature. The initial and advanced configurations are the same than those from Figure 1.

jumped from "particle" without microstructure to clusters with it, and that this microstructure is caused by interactions and temperature.

2.3. The Effect of Range and Intensity of the Potential

Notice that in the Metropolis algorithm the probability for the effectivization of a movement with a positive variation of the potential δU is given by $e^{-\delta U/kT}$, and that for a square potential δU is proportional to the difference between the number of particles in the range of the potential after the movement and before the movement. This difference is, for short movements, of small order, as the number of particles on the perimeter of the range. We set as a parameter the number $\mu = \Delta/kT$, where Δ denotes the intensity of the pair potential, and we test the μ values 1.0, 0.1, 0.01. There is a significant difference in the behaviour of our configurations with respect to the intensity μ, depending on the range of the potential.

All the examples below are obtained with 500 cycles of the Metropolis algorithm. Let us consider a length unity u. Then we work with a hard-core exclusion distance of 3 u. For moderate ranges ($r = 10$ u), there is a strong clustering effect for $\mu = 1.0$, thus giving

lower dimensions (see Fig. 3). (notice that the values tested for the parameters μ and r are consistent, in scale, with a rough approximation of liquids with van der Waals interactions, where the range of attraction is in the order of some interatomic distances and the pair intensity in the order of kT). But for longer ranges ($r = 20$ u), the clustering effect on dimension is negligible, and we find instead a remarkable ordering effect for $\mu = 1.0$ (we also see this effect starting from a random initial configuration, *i.e.*, this is not a consequence of the initial regularity). (see Fig. 4). We think that this last effect is rather artificial, due to the finite size and the rigidity of the system, but we have not obtained a complete explanation yet. For shorter ranges ($r = 7$ u), the clusters are smaller and there is a stronger random effect, and we obtain again a dimension $d_f = 1.74$ for $\mu = 1.0$, $\phi = 0.09$ (see Fig. 5). We show some evidence in the dimensions of Table I.

This clustering effect of the interaction potential contributes at low concentration to the correlation length, but near the percolation threshold the geometrical clustering due to contiguity prevails (see Fig. 6), and for density $\phi = 0.15$ we obtain $d_f = 1.74$ for $\mu = 1.0$ and $d_f = 1.77$ for $\mu = 0.1$.

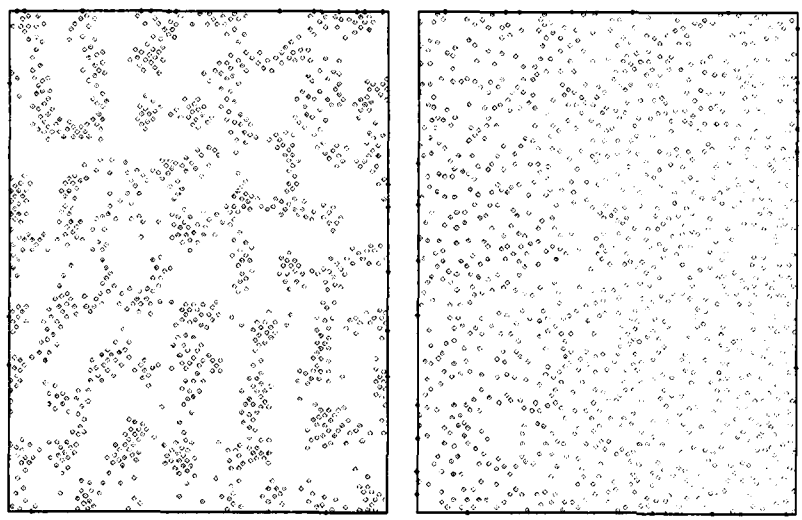

FIGURE 3 The clustering effect of intensity. $\mu = 0.1$ (left), $\mu = 0.1$ (right). $\phi = 0.09$, $r = 10$ u.

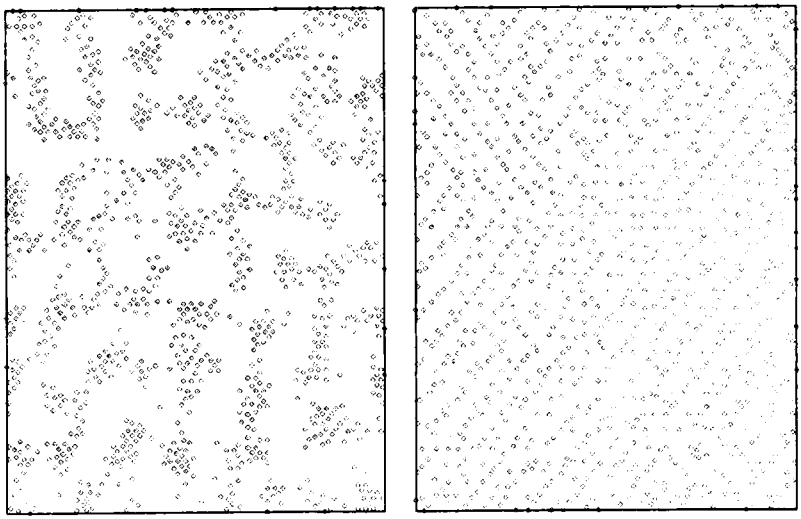

FIGURE 4 The variation in the effect of intensity due to range (I): $r = 10$ u (left), $r = 20$ u (right). $\phi = 0.09$, $\mu = 1.0$. Notice the remarkable regularity of the configuration on the right.

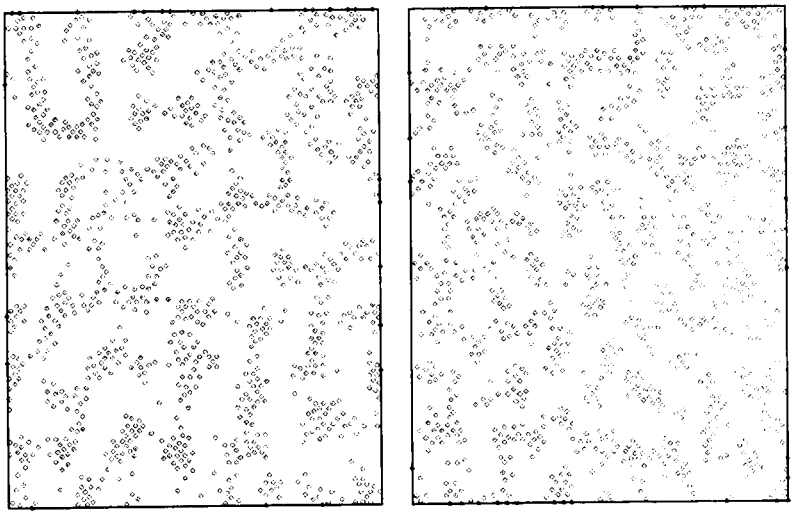

FIGURE 5 The variation in the effect of intensity due to range (II): $r = 10$ u (left), $r = 7$ u (right). $\phi = 0.09$, $\mu = 1.0$.

TABLE I Sensitivity of box-counting dimension to clustering. $r = 10$ u (left): strong clustering effect due to interactions for $\mu = 1.0$ (see Fig. 3). $r = 20$ u (right): the differences in the dimension due to the potential are negligible (see Fig. 4)

$\mu\backslash\phi$	0.07	0.09	0.11	$\mu\backslash\phi$	0.07	0.09	0.11
1.0	1.68	1.68	1.68	1.0	1.76	1.78	1.77
0.1	1.75	1.77	1.77	0.1	1.77	1.77	1.77
0.01	1.76	1.76	1.76	0.01	1.77	1.76	1.76

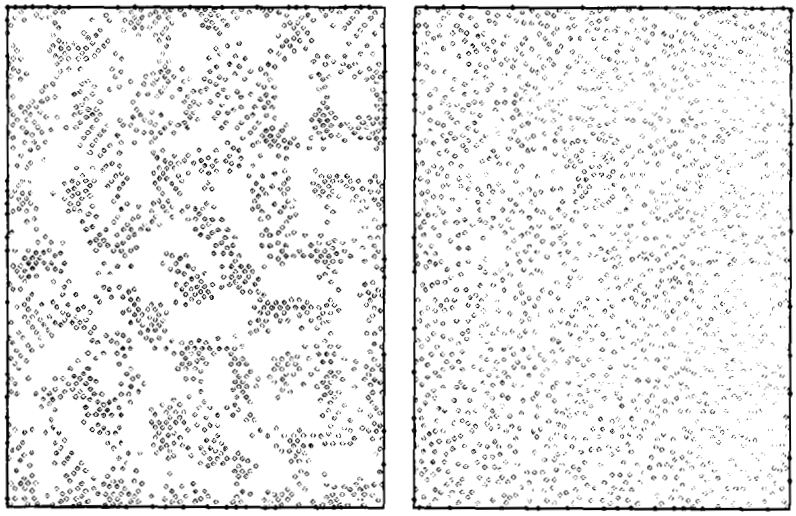

FIGURE 6 The interplay between the interaction and the percolation effect. $\mu = 1.0$ (left), $\mu = 0.1$ (right). $\phi = 0.15$, $r = 10$ u.

3. CONCLUSIONS

We showed in this work how the scaling behaviour of concentration, described globally by the box-counting fractal dimension, and a detailed analysis of the sources of its variation, contribute to the description of the interplay of diverse factors during the clustering processes below the percolation threshold. Thus, we showed

1. The artificial random effect alters greatly the computation of dimensions, and should be considered. We give a working solution to this problem, but it deserves further analysis.

2. The comparison of dimensions *via* their computation as slopes gives a good insight for the analysis of the contribution of different factors to the clustering phenomena: the breakpoints in the data curves are strongly indicative of two interplaying correlation lengths.
3. The clustering effect due to interactions at low densities depends strongly on the range of the potential. For moderate ranges, strong clustering, whereas for long and short ranges this effect becomes negligible, with different geometrical causes.
4. The clustering effect of interactions alters the scale in the percolation effect, where the particle scale is replaced by the slowly increasing correlation length of the interaction clusters. The geometrical effect of percolation and its rapidly increasing correlation length prevails near the threshold, as the universality argument predicts.

References

[1] Allen, M. P. and Tildesley, D. J. (1987). Computer Simulation of Liquids, Clarendon Press, Oxford.
[2] Bug, A., Safran, S., Grest, G. and Webman, I. (1985). Do interactions raise or lower a percolation threshold?, *Physical Review Letters*, **55**, 1896–1899.
[3] Bunde, A. and Havlin, S. (1991). Percolation I, in Fractals and Disordered Systems, Springer-Verlag, New York-Heidelberg, pp. 51–95.