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Original Research Paper

PERCOLATION TRANSITION AND TOPOLOGY

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ABSTRACT

A number of bidimensional random structures with increasing densities are simulated to explore possible links between Euler-Poincaré characteristic (EPC), or connectivity, and percolation threshold. For each structure model, the percolation threshold is compared with a number of typical points (extrema, zero crossings...) of the EPC curve. From these exercises, it can be concluded that the percolation threshold cannot be generally predicted using the evolution of the EPC.

Keywords: Euler-Poincaré characteristic, percolation threshold, topology.

INTRODUCTION

Consider a binary random set, defined in a 2D or 3D field, whose structure evolves and gradually densifies by successive unions of simple geometric objects (square, disk, triangle, ...) or morphological transformations (dilation, closure, ...). Initially, the structure consists of isolated objects. Then, as densification proceeds, it becomes more and more connected till it covers the whole field. When one structure evolves from a set made of isolated objects to a fully interconnected set, a percolation transition occurs which is expressed by an abrupt change from an «insulating» state to a «conducting» one (Ottavi *et al.*, 1978). Percolation is said to take place whenever there exist points of two opposite edges of the rectangular field (two opposite planes of the field for 3D case) that belong to the same connected component. This occurs for a minimal phase proportion that depends on the simulation considered. In other words, this minimal proportion is random. However, its distribution becomes less and less dispersed and tends to be supported by a point as the simulation field becomes infinitely large. This point support is called the percolation threshold. A question thus arises: is there a structural feature that could help to predict this percolation threshold? Percolation is clearly driven by the topology of the structure. This topology can be described by several attributes, among which the Euler-Poincaré characteristic (EPC) (Hadwiger, 1957) can be easily assessed.

The relationship between the topology of the structure and the percolation is illustrated on a simple example presented in Fig. 1. As more and more connections are added to the structure, the topology is changed, which modifies its EPC. Simultaneously, the filling of the phase is facilitated and the proportion of the phase invaded by the fluid increases.

Accordingly, the aim of this work is to examine the possible link between the percolation thresholds and the EPC (denoted as Nd, d indicating the space dimension in which the characteristic is defined). These links will be sought for several simulated densifying structures.

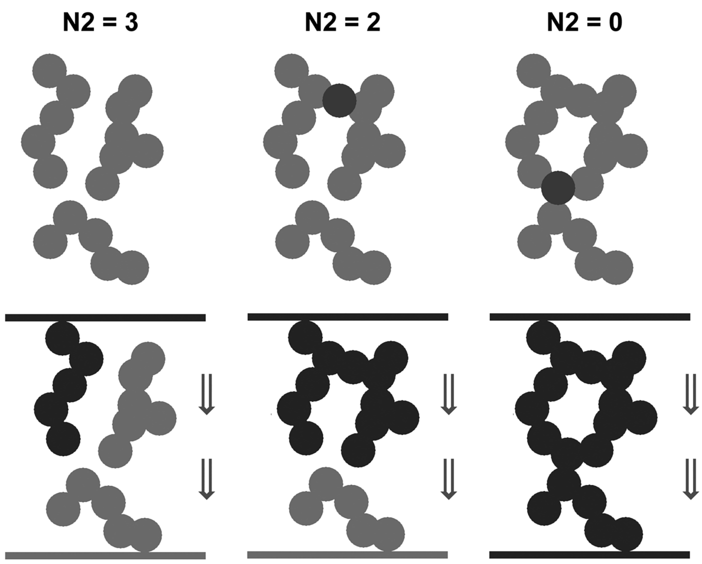

Fig. 1. *(Top) An increase of the number of connections modifies the topology of the phase which, in turn, leads to a decrease of the values of the EPC (N2). (Bottom) As the black phase is getting more and more connected, its invasion by a fluid (from the top to the bottom of the field) is more and more complete.*

MATERIALS AND METHODS

As EPC measurements are required, it is advantageous to work in discrete space which implies the choice of a digitization grid. As far as the percolation is studied, the connectivity of the grid, *i.e.*, the number of neighbors of each point should not modify the propagation within the structures themselves.

Taking those considerations into account, the experimental procedure is devised as follows. The simulations are carried out on a hexagonal 2000*2000 grid. The field size is taken 100 times larger than the objects to reduce statistical fluctuations. The simulations are of two types: i) random implantation of increasing numbers of points followed by dilations or closures ii) random implantation of increasing numbers of digitized objects such as squares, square crowns, crosses, triangles... (in the case of deterministic objects, the realizations obtained can be seen as realizations of a Boolean model with increasing intensity). For each structure, we evaluate (i) its compacity that is the proportion of the field occupied by the phase of interest and (ii) the invaded proportion that is the proportion of the phase invaded by geodesic propagation (Lantuéjoul and Beucher, 1981) from markers situated on one edge of the field. Suppose that percolation takes place. Then we estimate the percolation threshold as the inflection point of the curve that gives the invaded proportion versus the compacity. Jouannot (1994) observed that this inflection point corresponds roughly to a 50% invasion of the phase of interest. She also showed that this estimation procedure is equivalent to that recommended by Stauffer (1985 and 2009).

This procedure makes it possible to define accurately the percolation threshold using a limited number of simulations. Moreover, the field size effect influences only the width of the transition zone around the percolation threshold (Karioris and Mendelson, 1981). In this work, the steepness of the transition observed in all cases (Figs. 2-10) ensures that this size effect is quite limited.

In 2D space, the simplest and most widely used grids are the square and the hexagonal ones. This latter grid has been chosen for its isotropy and for its unambiguous connectivity. The six equidistant neighbors of a given point ensure propagation with maximal isotropy. In the case of a square grid, the connectivity of the grid can be arbitrarily defined as either four or eight. This is a major drawback for propagations: the percolation threshold of this grid uniformly filled with points corresponds to the values 0.59 for the 4-connectivity and 0.41 for the 8-connectivity (Fig. 2). Anyway, it should be pointed out that the difference between grids and their connectivity tends to vanish as the structure is filled with bigger and bigger monosized objects (Fig. 2). In that case, the results obtained are the same, irrespectively of the underlying grid.

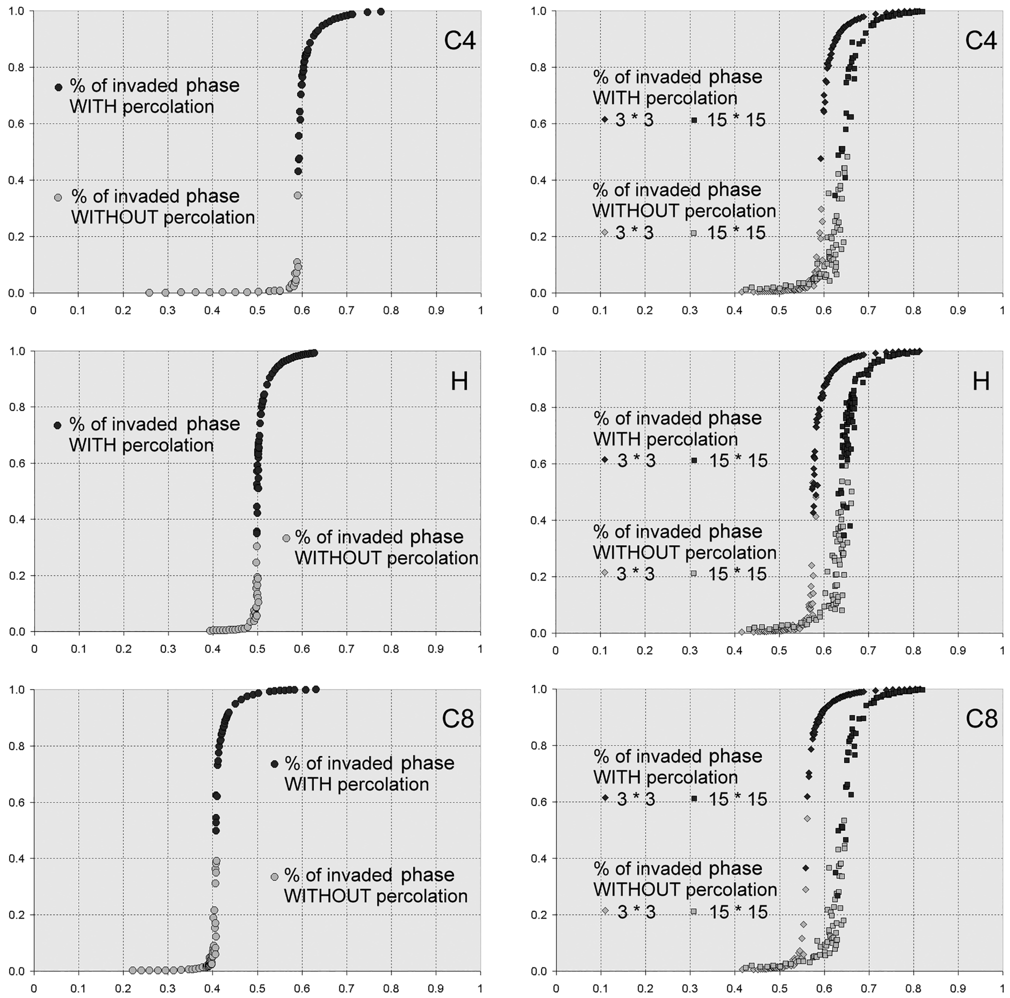

Fig. 2. *(Left) Propagations through increasing numbers of points uniformly distributed on 2000*2000 grids using a 4-connectivity square grid (top), 6-connectivity hexagonal grid (middle) or 8-connectivity square grid (bottom) lead to three different percolation thresholds. (Right) Propagations through increasing numbers of monosized squares (3*3 or 15*15) uniformly distributed on 2000*2000 grids using a 4-connectivity square grid (top), 6-connectivity hexagonal grid (middle) or 8-connectivity square grid (bottom) lead to the same percolation threshold only for the 15*15 squares. For all curves, the percentage of invaded area is plotted as a function of the compacity*

RESULTS AND DISCUSSION

All results are represented versus the compacity of the structure (X-axis). Regarding the EPC graphics, each point is assigned either N1 (1D) or N2 (2D) (Y-axis) that are respectively related to the perimeter and the curvature of the interface between the two phases. Regarding the percolation graphics, each point is assigned the maximum value of the percentage of phase invaded by the geodesic propagation (Y-axis). Full or hollow patterns are used depending on whether percolation has already taken place or not.

During the evolution of structures, the curves representing the topological parameters as a function of the compacity exhibit singular points such as extrema, zeros and inflection points. In what follows, a relationship between one of these singular points and the percolation threshold is investigated.

PERCOLATION THRESHOLD AND EPC: SEVERAL COINCIDENCES

For a uniform implantation of increasing numbers of 15*15 squares, the percolation occurs at a compacity close to 0.63 (Fig. 3).

This percolation threshold coincides with the compacity at which N1 reaches its maximum and N2 vanishes. These coincidences are also observed in Fig. 4 when the hexagonal grid of the simulation field is progressively filled by uniform points. In this case, the percolation transition is observed for a compacity equal to 0.5 which is also that of the inflection point of N2. Nevertheless, this coincidence is not observed for a uniform implantation of points on a square grid.

To go a step further, we attempt to extend the validity domain of the results by using more sophisticated structures. The previous simulations of points are easily but deeply modified by morphological transformations (Jouannot and Jernot, 1993).

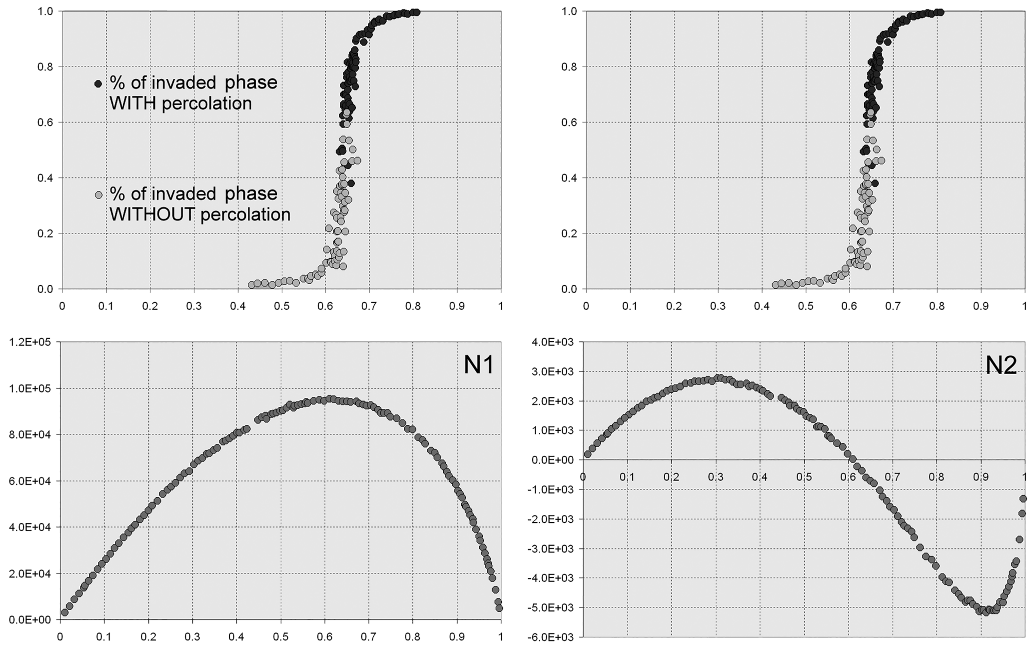

Fig. 3. *Increasing numbers of 15*15 squares uniformly placed on a hexagonal 2000*2000 grid: the curves depicting the evolution of the topology and the percolation process are compared as a function of the compacity.*

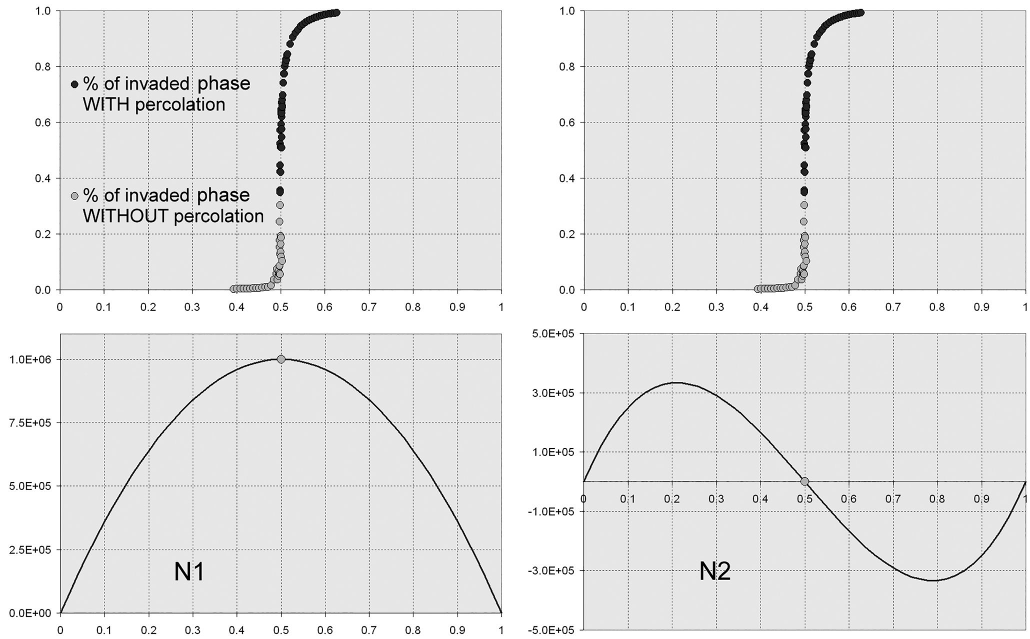

Fig. 4. *Increasing numbers of points uniformly distributed on a hexagonal 2000*2000 grid: a coincidence is observed between the maximum of N1, the zero and the inflection point of N2 and the percolation threshold.*

PERCOLATION THRESHOLD AND EPC: A SINGLE COINCIDENCE

The structures obtained from an increasing number of points uniformly distributed on the grid can be easily dilated or closed. Two such 2D examples are given in Figs. 5 and 6.

The coincidence with the zero value of N2 is no longer observed once the population of points has been morphologically transformed. Nevertheless, it can be seen in Figs. 5 and 6 that the percolation transition occurs at a compacity close to that of the maximum of N1. Such a link has already been observed not only in 2D, but also in 3D space with the two extrema of N2 for dilated or closed structures built on a 100*100*100 face-centered-cubic grid (Jouannot *et al.*, 1995). Some experimental observations of this coincidence are gathered in Table 1.

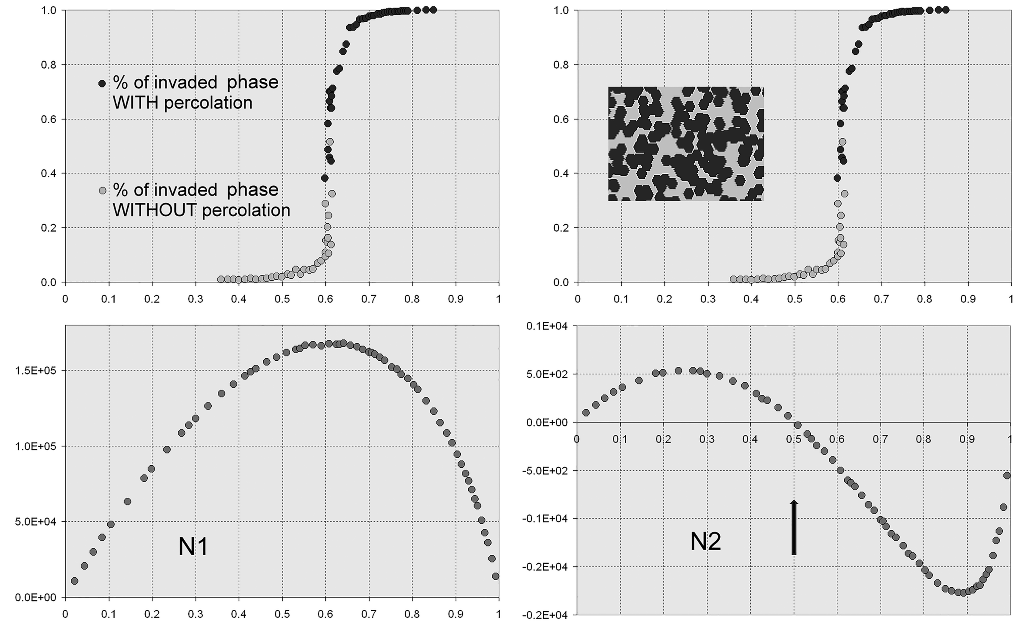

Fig. 5. *Structures obtained by applying a dilation of size 5 on increasing numbers of points uniformly distributed on the grid. A coincidence is observed between the percolation threshold and the maximum of N1 but no longer with the zero value of N2 (arrow).*

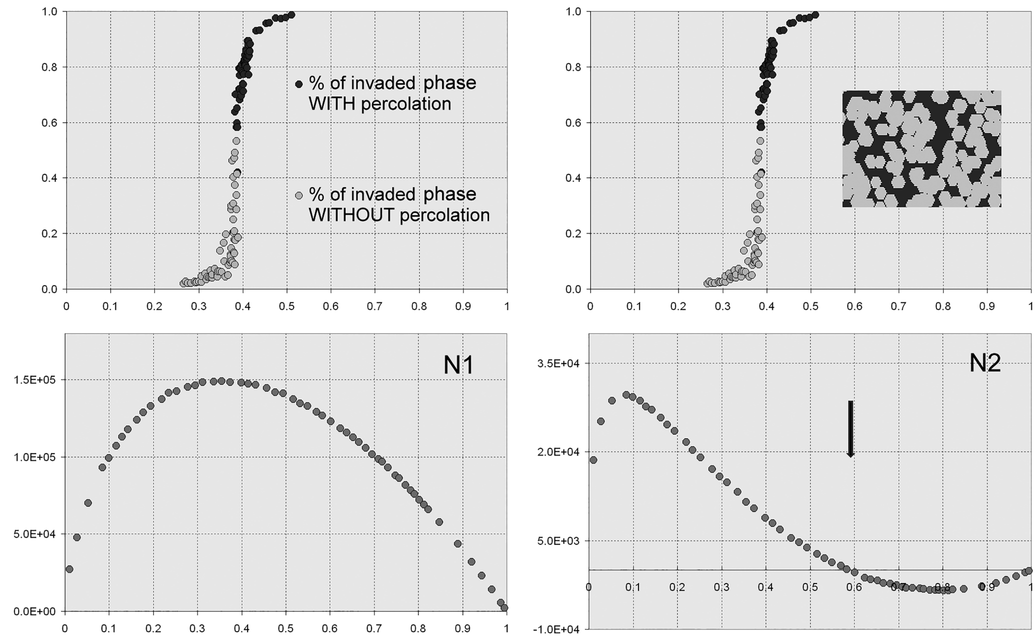

Fig. 6. *Structures obtained by applying a closure of size 5 on increasing numbers of points uniformly distributed on the grid. A coincidence is observed between the percolation threshold and the maximum of N1 but no longer with the zero value of N2 (arrow).*

Table 1. *Percolation thresholds and singular values of EPC for dilated and closed 2D or 3D structures.*

	Extremum of N1	Percolation threshold
2D dilated structures	0.61	0.61
2D closed structures	0.37	0.38

	Extrema of N2	Percolation thresholds
3D dilated structures	0.27 0.90	0.25 0.92
3D closed structures	0.07 0.72	0.07 0.72

As already mentioned, this coincidence was also observed for a uniform implantation of increasing numbers of squares. Is it still valid when the objects are not convex?

PERCOLATION THRESHOLD AND EPC: NO COINCIDENCE

Two kinds of non-convex monosized objects are used in the simulations: square crowns (outer width 21, thickness 3) and crosses (width 21, thickness 3). Such objects are gradually and uniformly distributed on the 2000*2000 hexagonal grid. The topological evolutions and the percolation results are presented in Figs 7 and 8.

When the structures are made up with square crowns, N2 exhibits only negative values and therefore the zero of N2 cannot obviously be linked to the percolation threshold. Moreover, it can be seen in Fig. 7 that the percolation threshold is far from the compacity value corresponding to the maximum of N1. In the case of crosses (Fig. 8), the percolation threshold is halfway between the zero value of N2 and the maximum of N1.

We can deduce from these results that the coincidence between the singular values of the EPC and the percolation threshold may not be observed for structures built from non-convex objects. We are then faced with the following question: are there any convex objects producing structures for which the same lack of coincidence is observed?

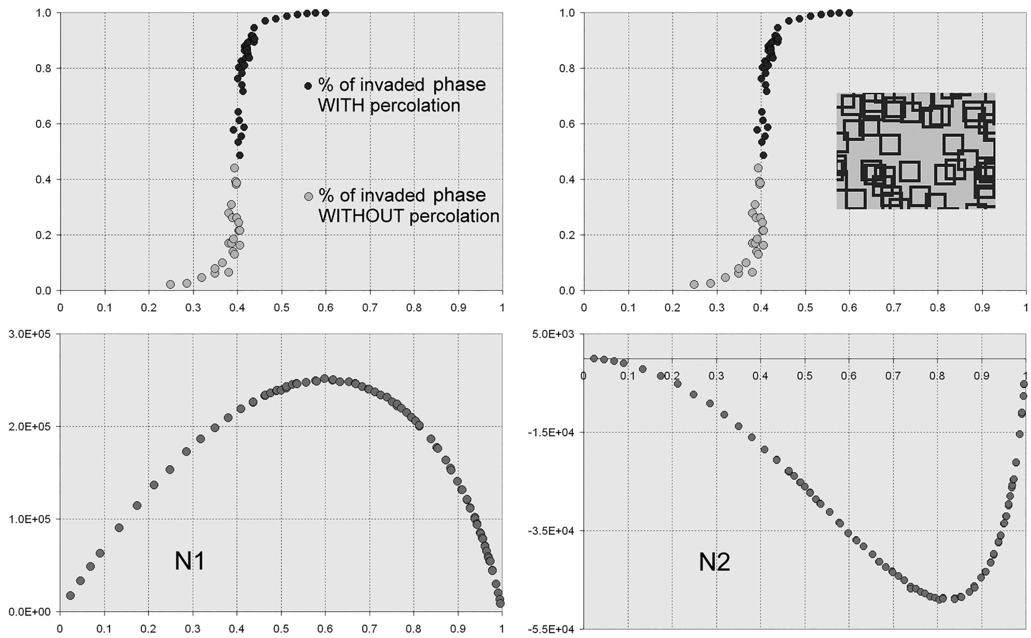

Fig. 7. *Increasing numbers of square crowns (outer width 21, thickness 3) are uniformly placed on a hexagonal 2000*2000 grid. The percolation threshold does not match with any of the singular points of the curves depicting the topological evolution of the structure.*

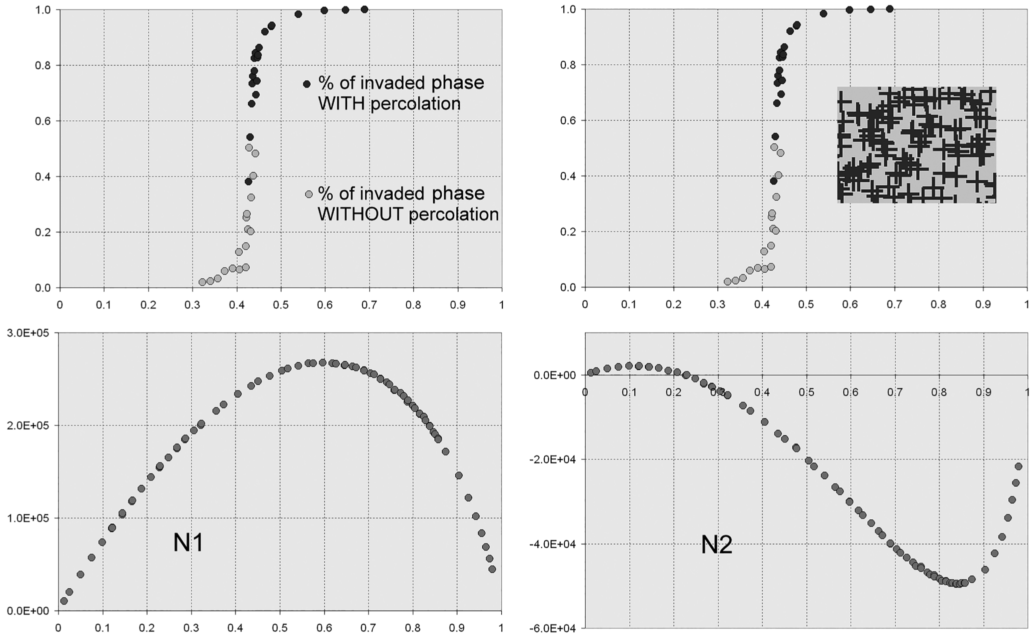

Fig. 8. *Increasing numbers of crosses (width 21, thickness 3) are uniformly placed on a hexagonal 2000*2000 grid. The percolation threshold does not match with any of the singular points of the curves depicting the topological evolution of the structure.*

SYNOPSIS

Up to now, we have seen on several examples that the zero value of N2 cannot be used to predict accurately the percolation threshold of 2D structures. Although this value is not very different from that of the threshold in a few cases (Bretheau and Jeulin, 1989) (Mecke and Wagner, 1991) (Mecke and Arns, 2005) (Neher *et al.*, 2008) (Miller *et al.*, 2010) (Levitz *et al.*, 2012), the above examples show that this is not generally true. As far as N1 is considered, the coincidence between its maximum and the percolation threshold seems to be more often encountered (Figs. 3 to 6) except for the structures built from non-convex objects (Figs. 7 and 8). But a counterexample can be found even for convex objects such as equilateral triangles.

Two kinds of simulations are compared in Fig. 9: the first one is made up with increasing numbers of uniformly placed uppointing triangles while the second one is made up with a half-half mixture of uppointing and downpointing triangles. An amazing comparison of the results is presented in this figure. Unexpectedly, we obtain two distinct curves for the percolation associated with two different thresholds but a unique curve for N1 with a single maximum.

What about the 3D space? The zeros of the 3D connectivity number, N3, were used to estimate the percolation thresholds (Jeulin and Moreaud, 2006) but in this space again the extrema of the 2D connectivity number, N2, provide better estimates of the percolation thresholds. This is illustrated on a simple example for which the EPC values can be exactly calculated: a face-centered-cubic grid uniformly filled with an increasing number of points. At first sight, it appears in Fig. 10 that the extrema of N2 are very close to the percolation thresholds, N2 playing the same role as N1 in 2D space (see also the coincidences concerning 3D dilated or closed structures in Table 1). Unfortunately, as can be seen in Table 2, the exact coincidence observed in 2D space (hexagonal grid) does not persist in 3D space.

Finally, from the equation of N3, one can check that the two inflection points of N3, exactly calculated, do not coincide with the two percolation thresholds on the f.c.c. grid (Table 2). Although it could have been an acceptable, but inaccurate, candidate on the basis of the results gathered in 2D space, the inflection point must then also be discarded.

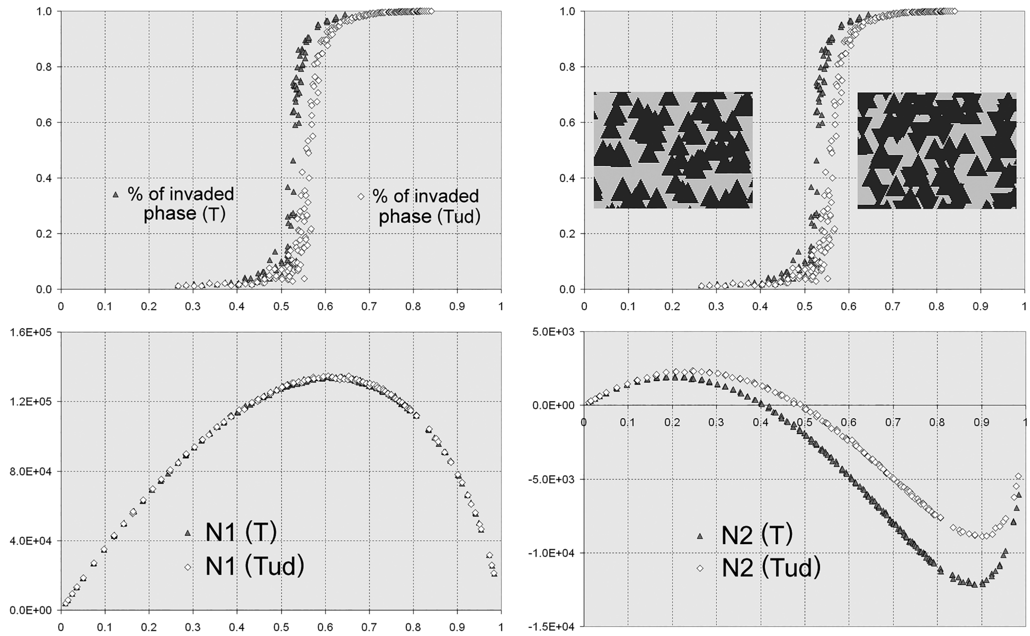

Fig. 9. *Two procedures are used to fill progressively the space with triangles (edge 20): uniform implantation of up pointing triangles (T) and mixture of half-half up and down pointing triangles (Tud). For these two simulations, two different percolation transitions are observed (upper curves). As far as the topological properties are concerned (lower curves), the thresholds correspond neither to the zeros of N2 nor to the compacity of the maximum of N1 for which a single curve is obtained.*

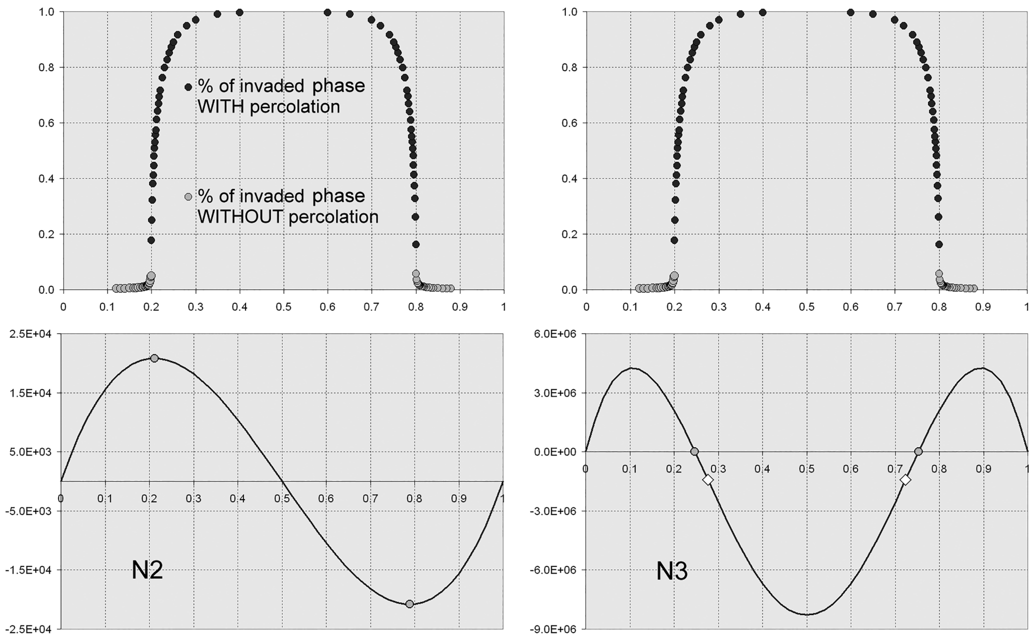

Fig. 10. *Increasing numbers of points uniformly distributed on a face-centered-cubic 500*500*500 grid (the natural 12-connectivity of the f.c.c. grid has been used for the propagations and the theoretical curves of the EPC represented here could have been obtained by sweeping the whole space with the rhomboedral unit of the f.c.c. grid). The compacities for which the two percolation thresholds occur are about 0.2 and 0.8 in the vicinity of the extrema of N2.*

Table 2. *Percolation thresholds and singular values of EPC for structures of points uniformly distributed on a hexagonal or on a face-centered-cubic grid.*

2D hexagonal grid			
Extremum of N1	Zero of N2	Inflection point of N2	Percolation threshold
0.500	0.500	0.500	0.5
3D face-centered-cubic grid			
Extrema of N2	Zeros of N3	Inflection points of N3	Percolation thresholds
0.211 0.789	0.247 0.753	0.276 0.724	0.2 0.8

CONCLUSION

Surprisingly, these simulations make it possible to conclude that the percolation threshold is generally not related to any singular point of the curves reflecting the evolution of the Euler-Poincaré characteristic of a structure. What can be inferred is then that there does not exist any direct link between the percolation threshold(s) of a structure and its topology.

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