Looking for a link between the microstructure and the percolation threshold

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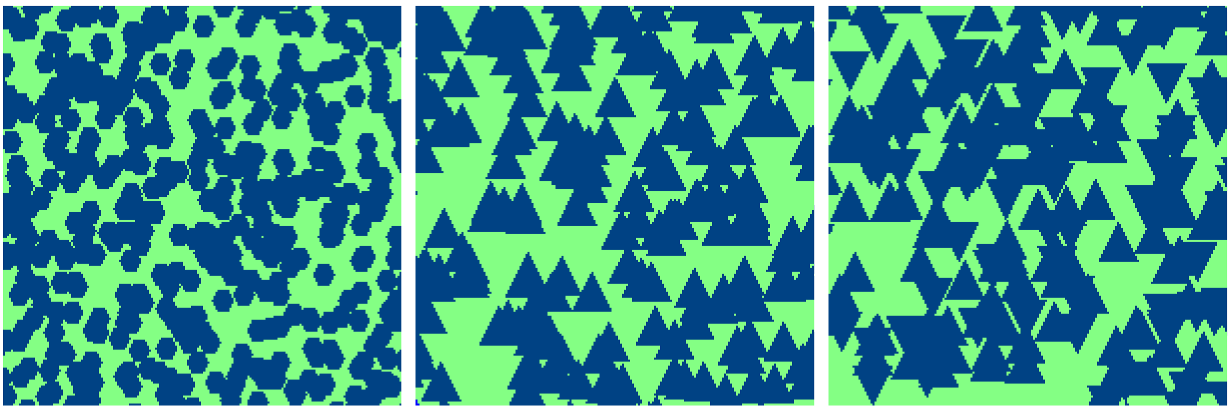
Introduction

Consider random binary 2D sets whose structure evolves and gradually densifies by successive unions of simple geometric elements (square, disk, triangle, ...) or morphological transformations (dilation, closure, ...). Initially, the structures consist of isolated elements. Then, they gradually connect, as densification proceeds, till forming a single set covering all the space. When one structure evolves from a set with only isolated elements to reach a fully interconnected set, a "percolation transition" occurs which is expressed by an abrupt change from an "insulating" state to a "conducting" one (Clerc et al., 1983). Then a question arises: "is there a structural feature that could make prediction of this percolation transition possible?" Percolation is clearly related to the topology of the structure. Such a topology can be described by several attributes, among which the Euler-Poincaré characteristic (EPC) (Hadwiger, 1957) can be easily assessed. Accordingly, the aim of this work is to examine the possible links between the EPC and percolation thresholds.

Simulations

Densification is quantified by the area fraction occupied by the phase of interest (also called compacity). For each compacity, the topological parameters, N1 (1D EPC) and N2 (2D EPC), respectively related to the perimeter and the curvature of the interface between the two phases are computed... During the evolution of structures, the curves representing these parameters exhibit remarkable points such as extrema, zeros and inflection points. Therefore, we tried to find a coincidence between any of these remarkable points and the percolation threshold. The simulations are carried out on a hexagonal 2000 * 2000 grid. The simulations are of two types: random implantation of increasing numbers of points followed by dilations or closures and random implantation of increasing numbers of elementary units such as solid or empty squares, crosses, triangles... Examples of simulations are given in Figure 1.



(a) (b) (c)

Figure 1. Simulated structures: uniform implantation of hexagons (a), up triangles (b), mixture of half up and half down triangles (c).

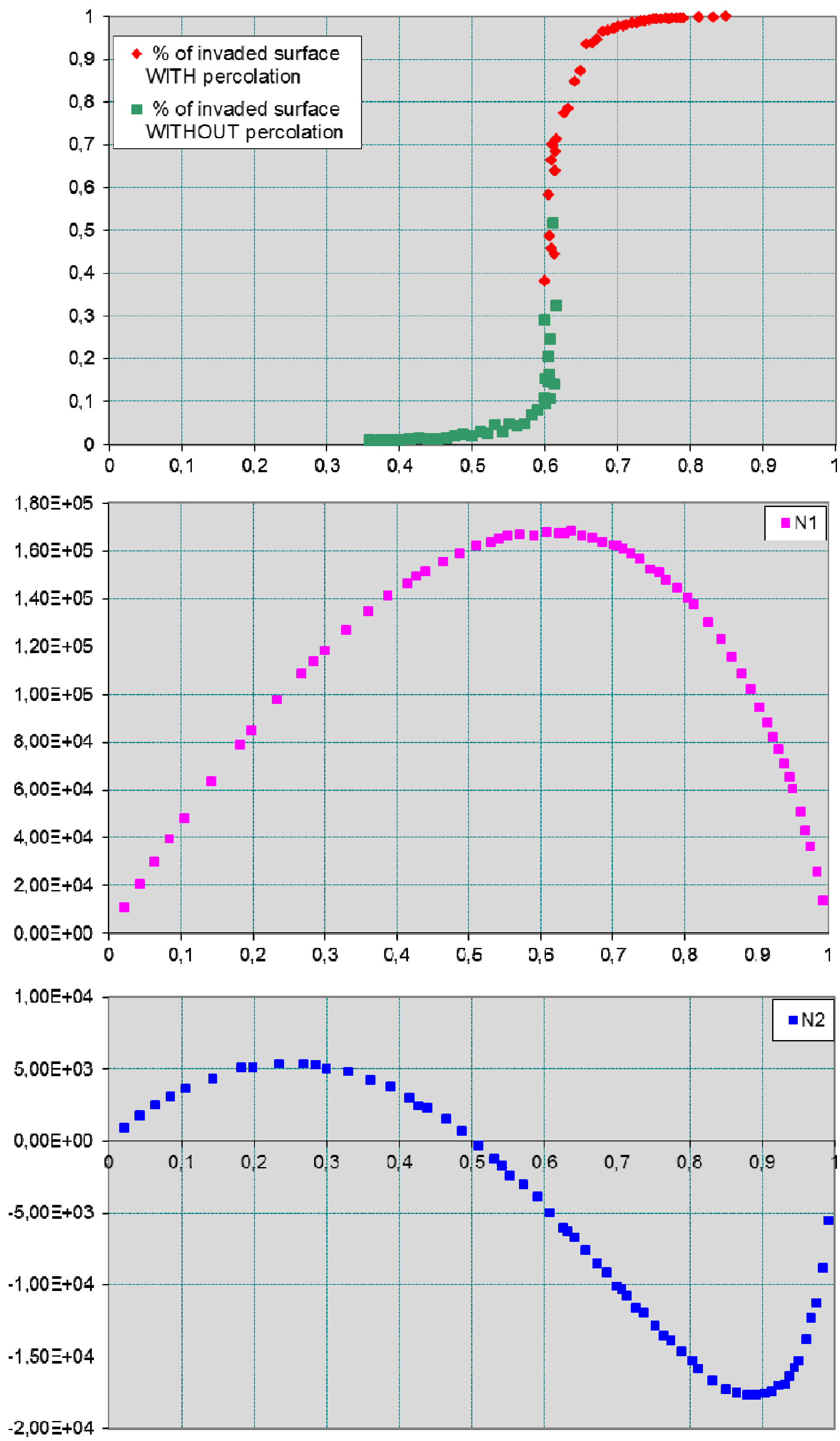


Figure 2. Uniform implantation of hexagons on a hexagonal grid. Increasing the number of hexagons allows a progressive filling of the space during which a percolation transition is observed (upper curve). The topological evolution of the densifying structure is followed through its EPC (lower curves) as a function of the compacity. A coincidence is observed between the percolation threshold and the compacity attained at the maximum of N1. Note that it differs from the zero of N2.

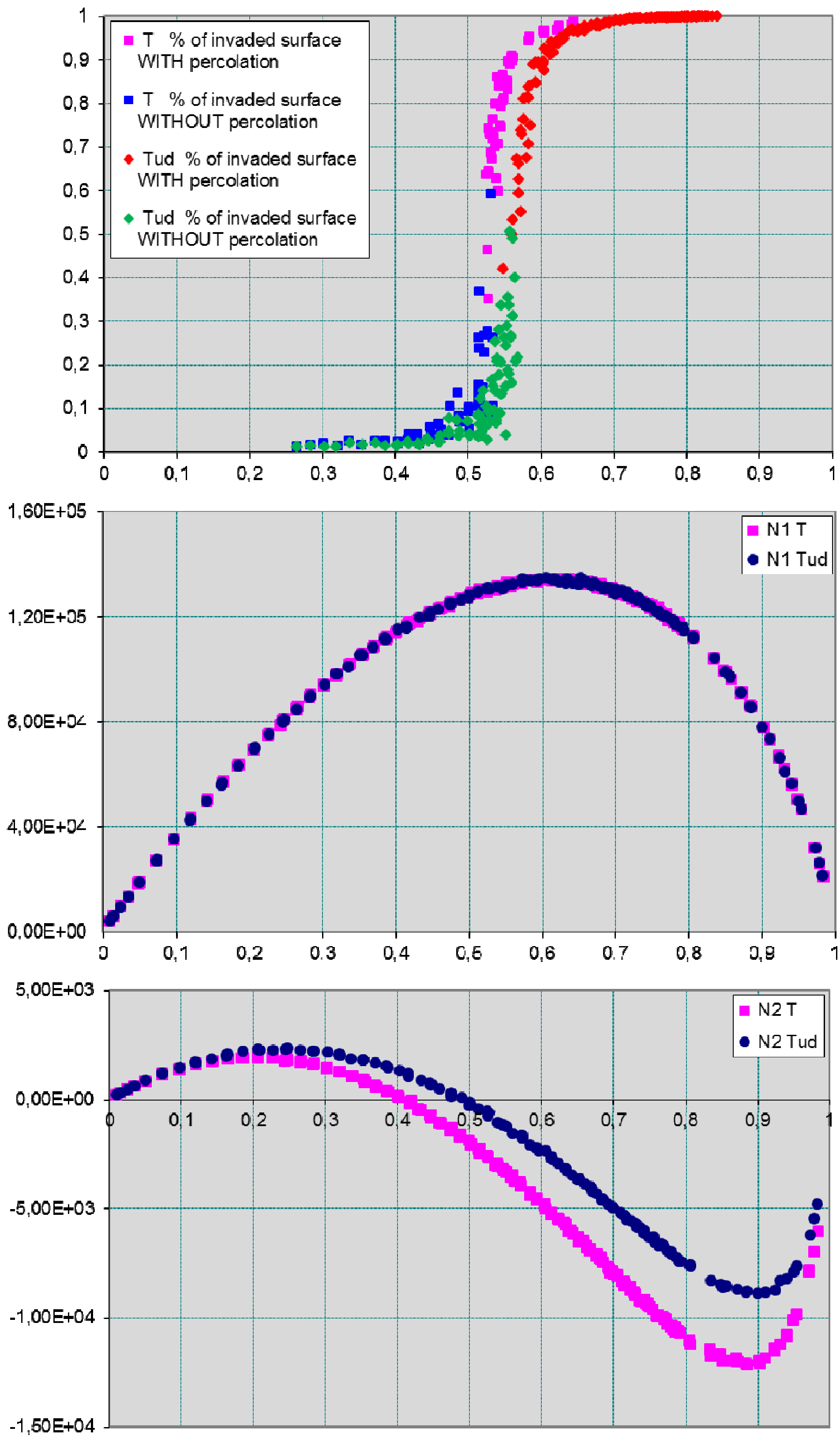


Figure 3. Two progressive fillings of the space with triangles: uniform implantation of up triangles (T) and mixture of half up and half down triangles (Tud). For these two simulations, two different percolation transitions are observed (upper curve). As far as the topological properties are concerned (lower curves), these transitions correspond neither to the zeros of N2 nor to the compacity value of the unique maximum of N1 for which a single curve is obtained.

The percolation threshold is assessed using the proportion of phase of interest invaded by a geodesic propagation (Lantuéjoul and Beucher, 1981). The markers of the propagation are located on the left edge of the field and we also checked whether the right edge of the field is reached (percolation through the field).

Results and Discussion

When the hexagonal grid of the simulation field is progressively filled by points, the percolation transition is observed for a compacity equal to 0.5. This value corresponds to the maximum of N1, the zero of N2 and the inflection point of N2 (Jernot and Jouannot, 1993). The coincidence observed between the compacity at those points and that of the percolation threshold is also valid for a uniform implantation of increasing numbers of elementary squares: in this case, the compacity is close to 0.63 (this is also observed using a square grid). The coincidence with the zero value of N2 is no longer observed when morphological transformations are performed on the set under consideration. This is illustrated in Figure 2 corresponding to dilated structures of points. Moreover, when the structures are made up with square boundaries, N2 exhibits only negative values and therefore the zero of N2 cannot obviously be linked to the percolation threshold. Nevertheless, it can be seen in Figure 2 that the percolation transition occurs close to the compacity of the maximum of N1. This link with the extremum of N1 in 2D space and the extrema of N2 in 3D space had already been observed for dilated or closed structures (Jouannot et al., 1995). But a counterexample can be found from two other simulations based on equilateral triangles. The first one is made up with increasing numbers of uniformly placed "up triangles" while the second one is made up with a 50-50 mixture of "up triangles" and "down triangles" (see Figure 1). An amazing comparison of these two simulations is presented in Figure 3. The same curve is obtained for N1 leading to a single maximum while two distinct curves for the percolation are associated with two percolation thresholds. Finally, we also have to reject the inflection point of N2. Although it could have been an acceptable candidate on the basis of all our results gathered in 2D space, it must also be discarded because the coincidence doesn't persist in 3D space. From the equation of N3 (Jernot and Jouannot, 1993) one can check that the two inflection points of N3 do not coincide with the two percolation thresholds on a f.c.c. grid uniformly filled by points.

Conclusion

Surprisingly, these simulations allow concluding that the percolation threshold is not linked to any remarkable point of the curves reflecting the topological evolution of a structure. What can be inferred is then that there does not exist any direct link between percolation thresholds and the Euler-Poincaré characteristic.

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