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LETTER TO THE EDITOR

Absence of universality in percolation models of disordered elastic media with central forces

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Abstract. We investigate the universality of scaling laws in elastic percolation networks with central forces. Near the percolation threshold p_{ce} the elastic moduli G vanish as $G \sim (p - p_{ce})^f$, and the correlation length ξ_e diverges as $\xi_e \sim (p - p_{ce})^{-\nu_e}$, where p is the fraction of active bonds. For bond, correlated bond and site percolation on a triangular network we estimate the ratio f/ν_e using Monte Carlo simulations and finite-size scaling analysis, and find $f/\nu_e \simeq 1.42$, 1.28 and 1.14, respectively. We also find a different value of ν_e for each of these percolation processes. Therefore, topological and mechanical properties of disordered media with central forces may not have universal properties, and may depend strongly on the microscopic details of the elastic media. These results may also have implications for other vector models of phase transition.

Elastic percolation networks and their topological and mechanical properties near the percolation threshold p_{ce} have recently received considerable attention. Such systems, which are relevant to a large class of disordered materials, such as gels, aggregates and composites, have been studied both theoretically and experimentally, and many new results have emerged. Jerauld (1985) and Feng and Sen (1984) studied a simple elastic percolation network, namely the central force (CF) model, which is essentially a network of simple springs in which only stretching forces are present. The percolation problem that was studied by these authors was a bond percolation (BP) process in which each spring is present with a probability p. The potential energy of the system is given by

$$E = \tfrac{1}{2} \sum_{\langle ij \rangle} [(\boldsymbol{u}_i - \boldsymbol{u}_j) \cdot \boldsymbol{R}_{ij}]^2 k_{ij} \tag{1}$$

where $\boldsymbol{u}_i$ and $\boldsymbol{u}_j$ are displacements of sites i and j, and $\boldsymbol{R}_{ij}$ a unit vector from site i to j. Here k_{ij} is a random variable which takes a finite value with probability p and is 0 with probability $1-p$, and essentially represents the elastic constant of the spring between i and j. This model is rotationally invariant and bears a close resemblance to various finite-element models in macroscopic stress analysis. It can be constructed by a finite-element discretisation of the Navier equations, in which one employs bilinear basis functions defined on an equilateral triangle and a Poisson ratio equal to $\frac{1}{3}$. Thus, this model may be considered an analogue of a three-dimensional solid in planar strain, pierced by cylindrical holes normal to the plane of strain. One can in a similar

manner construct a three-dimensional version of the model on a FCC or BCC network. Near the percolation threshold, the elastic moduli G of the system appear to obey the following power law:

$$G \sim (p - p_{ce})^{f} \tag{2}$$

where f is a critical exponent. It was established by Jerauld (1985) and Feng and Sen (1984) that p_{ce} is much larger than p_c, the connectivity (or conductivity) threshold. For example, for simple-cubic networks in any dimension one has the peculiar property that $p_{ce} = 1$. Therefore, a meaningful study of this problem is restricted to certain networks, e.g. triangular and BCC networks, and for the triangular network one has (Jerauld 1985, Sahimi and Goddard 1985, Lemieux *et al* 1985) $p_{ce} \simeq 0.65$ for BP, as compared with $p_c = 0.347$. Numerical simulations of Feng and Sen (1984) also indicated that f may be much larger than t, the critical exponent of conductivity. Day *et al* (1986) have shown that the *topological* properties of percolation clusters in the CF model differ considerably from those of ordinary percolation clusters. For the CF model a correlation length ξ_e can be defined which appears to diverge as p_{ce} is approached:

$$\xi_e \sim (p - p_{ce})^{-\nu_e} \tag{3}$$

where (Sahimi and Goddard 1985, Lemieux *et al* 1985, Day *et al* 1986) $\nu_e \simeq 1.1$ for two-dimensional systems, whereas the correlation length exponent of ordinary percolation is $\nu = \frac{4}{3}$. The most accurate estimate of f for two-dimensional systems appears to be (Sahimi and Goddard 1985, Lemieux *et al* 1985) $f/\nu_e \simeq 1.45$, as opposed to $t/\nu \simeq 0.97$. The CF model has also been studied within an effective-medium approximation (EMA) by several authors (Jerauld 1985, Feng *et al* 1985, Garboczi and Thorpe 1985a, b, 1986, Thorpe and Garboczi 1987) and it appears that the EMA is very accurate for describing the CF model.

The main goal of this letter is to test the idea of universality for the CF model. For ordinary percolation, the critical exponent t is universal, and it depends only on the dimensionality of the system (except for a special class of continuous systems). It does not depend on the type of the network, or whether one considers BP or site percolation (SP). However, it is not clear that f should also be universal, because in elastic percolation networks the contribution of each cluster depends not only on its connectivity (as in the case of conductivity or, more generally, *scalar* problems), but also on its shape and the kind of microscopic force law that one uses. Prunet and Blanc (1986) and Wang (1988) have studied the critical properties of *rigid site and bond animals*, i.e. large elastic clusters that are formed in the CF model *below* p_{ce}. Their results indicate that site and bond animals may be described by different scaling laws. Garcia-Molina *et al* (1988) have studied the effect of the ratio of the two Lamé constants (in the Navier equations) on the elastic properties of percolation networks, and have found that this ratio strongly affects the critical behaviour. However, the universality of BP and SP in elastic percolation networks and the possible dependence of the critical exponents on the microscopic details of the system have not been investigated before. In this letter we study this for the CF model because it has a well established link with real continuous systems, whereas elastic percolation systems in which both the central and bond-bending forces are present (Kantor and Webman 1984, Feng and Sahimi 1985, Zabolitzky *et al* 1986) do not seem to have such correspondence with continuum equations, although they have been argued to be better models for real systems.

We have studied the CF model in SP and BP on a triangular network. Site percolation on a triangular network has been previously studied by Thorpe and Garboczi (1987) within an EMA, and by numerical simulations. However, the critical behaviour of G or ξ_e was not studied by these authors. We have also studied the CF model within a correlated-bond percolation (CBP) process. In this model, which was originally proposed by Kirkpatrick (1973) for studying of hopping conduction in disordered materials, each site is assigned a random number S_i uniformly distributed in $(-1, +1)$. Random numbers S_{ij} for the bonds connecting sites i and j are calculated via $S_{ij} = \frac{1}{2}(|S_i|+|S_j|+|S_i - S_j|)$. All bonds with $S_{ij} > \Delta$ are removed, where Δ is some selected limit. It is easy to show that the fraction $p(\Delta)$ of remaining bonds is given by

$$p(\Delta) = \begin{cases} \frac{3}{4}\Delta^2 & 0 \leqslant \Delta \leqslant 1 \\ \Delta - \frac{1}{4}\Delta^2 & 1 \leqslant \Delta \leqslant 2. \end{cases} \tag{4}$$

We first determined the percolation threshold p_{ce} for SP and CBP in the CF model. In order to do this, we used finite-size scaling analysis (FSSA) according to which (Levinshtein *et al* 1976)

$$p_{ce}(L = \infty) - p_{ce}(L) \sim L^{-x} \tag{5}$$

where $x = \nu_e^{-1}$, and $p_{ce}(L)$ is the effective percolation threshold of a network of linear size L. Therefore, we used various network sizes, ranging from $L = 10$ to $L = 45$. For each network size we determined the nodal displacements by minimising E with respect to $\boldsymbol{u}_i$ and solving the resulting set of linear equations by Gaussian elimination; from the solution of this set we determined G. We then used many realisations and averaged the results; table 1 presents the statistics of our simulations. Non-percolating clusters were discarded from our simulations, and the numbers in table 1 refer to the number of percolating configurations. Thus, the total number of realisations (percolating or not) were much larger than those shown in table 1. In figure 1 we present the variations of $p_{ce}(L)$ with L for SP. A fit of the data to equation (5) yields

$$p_{ce} \simeq 0.71 \pm 0.01 \qquad \nu_e \simeq 0.94 \pm 0.05 \qquad \text{for SP.} \tag{6}$$

It is interesting to note that p_{ce} is well represented by $(2)^{-1/2}$.

Next, we determined p_{ce} for CBP. We first used a mean-field-like argument to estimate p_{ce}. The average number N_c of bonds at each site of the network in BP is $N_c = zp$, where $z = 6$ is the coordination number of the triangular network. Thus, at p_{ce} of BP one has $N_c \simeq 6 \times 0.65 = 3.9$. On the other hand, in CBP one has $N_c = zp/\Delta$ which, in view of (5), means that $N_c = \frac{9}{2}\Delta$. If we assume that N_c at p_{ce} is essentially the same for both BP and CBP, we obtain $\Delta(p_{ce}) \simeq 0.87$, which means that $p_{ce} \simeq 0.57$ for CBP on the triangular network. In figure 1 we also present the dependence of $p_{ce}(L)$ on L for CBP, from which we obtain

$$p_{ce} \simeq 0.58 \pm 0.01 \qquad \nu_e \simeq 0.90 \pm 0.05 \qquad \text{for CBP} \tag{7}$$

Table 1. Number of realisations for each network size L for various percolation models.

L	10	15	20	25	30	35	40	45
Bond percolation	300	240	200	160	100	100	100	60
Site percolation	300	300	200	200	—	120	—	120
Correlated bond percolation	300	300	700	200	—	120	—	100

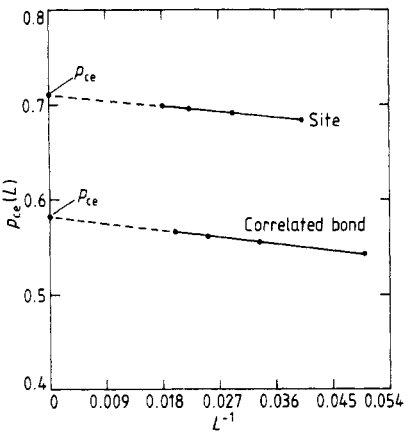

Figure 1. Dependence of $p_{ce}(L)$ on the network size L for site and correlated bond percolation. Full circles are the Monte Carlo data, and full lines are the best fit to equation (5).

which is in agreement with our mean-field estimate. In fact, if we use the prediction of EMA, $N_c(p_{ce}) = 4$, we obtain $p_{ce} = \frac{16}{27} \simeq 0.59$, which is also in agreement with (7). Note that for BP one has (Sahimi and Goddard 1985, Lemieux *et al* 1985) $\nu_e \simeq 1.1$. In figure 2 we present the dependence of the bulk modulus G on $p(\Delta)$ in CBP. For $\Delta < 1$ ($p < 0.75$), this problem is more similar to a SP model, because a bond would not be removed if and only if $|S_i| < \Delta$ *and* $|S_j| < \Delta$. This is also clear from figure 2. For $p < 0.75$, the variation of G with p has a distinct curvature, which is typical of a SP model (in BP, only very close to p_{ce} one observes a distinct curvature).

To estimate f, we again used FSSA according to which

$$G \sim L^{-y}(1 + ag_1(L) + bg_2(L)) \tag{8}$$

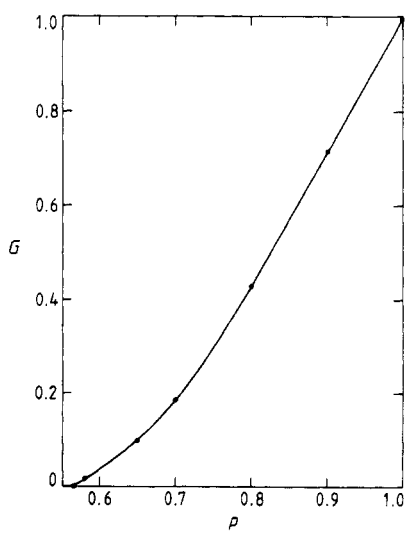

Figure 2. Variation of the bulk modulus G with the fraction p of active bonds in the correlated bond percolation. Full circles are the Monte Carlo data.

for a network of linear dimension L at p_{ce}. Here $g_1(L)$ and $g_2(L)$ represent, respectively, the leading non-analytical and analytical correction terms to scaling, f/ν_e, and a and b are constant. Various forms of $g_1(L)$ and $g_2(L)$ were tried in order to obtain the best fit to the data. We found that the best fit in all cases is provided by

$$g_1(L) = (\ln L)^{-1} \qquad g_2(L) = L^{-1}. \tag{9}$$

Using these, we obtained (see figure 3)

$$y = f/\nu_e = \begin{cases} 1.42 \pm 0.04 & \text{BP} \\ 1.28 \pm 0.04 & \text{CBP} \\ 1.14 \pm 0.04 & \text{SP.} \end{cases} \tag{10}$$

The difference between the results for various models is large enough that we believe our results are conclusive evidence that there is no universality for the critical exponents that characterise the CF model. However, we should mention that our estimates of ν_e for various models are less accurate than those of f/ν_e. We also found that corrections to scaling affect significantly the estimates of f/ν_e. For example, if we neglect $g_1(L)$ and $g_2(L)$, we obtain $f/\nu_e \simeq 1.03$ for SP. In all cases the values of a and b in equation (8) were of the order of unity, as they should be. For example, we found $a \simeq 2.4$ and $b \simeq 2.9$ for BP. The results for SP and CBP also indicate that, at least for the CF model, it is possible that the elasticity exponents for certain percolation processes can be *less* than the conductivity exponent t. However, *the ratio* f/ν_e which, for *finite* systems, is the proper quantity, is always *greater* than t/ν.

In summary, we have presented the first conclusive evidence that various percolation processes in the CF model are *not* characterised by universal scaling laws. The critical exponents appear to depend on the microscopic details of the system. Whether elastic networks with both the central and bond-bending forces exhibit the same type of non-universal behaviour is still an open question. If so, such models may not be as general as they have been thought to be. Our results may also have implications for

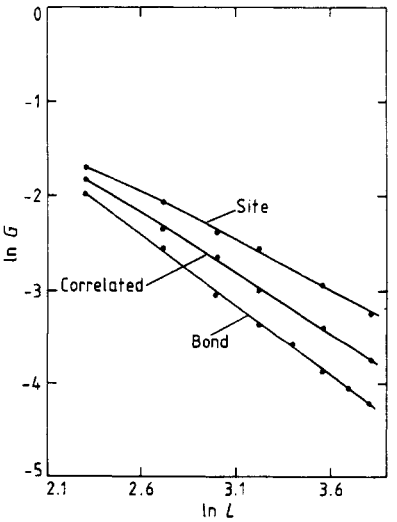

Figure 3. Dependence of ln G on ln L at p_{ce} for various percolation models. Full circles are the Monte Carlo data, and the curves are the best fit to equation (8).

other vector models of phase transition such as the Heisenberg model. These matters will be discussed in a future paper.

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References

Day A R, Tremblay R R and Tremblay A-M S 1986 *Phys. Rev. Lett.* **56** 2501
Feng S and Sahimi M 1985 *Phys. Rev.* B **31** 1671
Feng S and Sen P N 1984 *Phys. Rev. Lett.* **52** 216
Feng S, Thorpe M F and Garboczi E 1985 *Phys. Rev.* B **31** 276
Garboczi E and Thorpe M F 1985a *Phys. Rev.* B **31** 7276
—— 1985b *Phys. Rev.* B **32** 4513
—— 1986 *Phys. Rev.* B **33** 3289
Garcia-Molina R, Guinea F and Louis E 1988 *Phys. Rev. Lett.* **60** 124
Jerauld G R 1985 *PhD thesis* University of Minnesota, Minneapolis
Kantor Y and Webman I 1984 *Phys. Rev. Lett.* **52** 1891
Kirkpatrick S 1973 *Rev. Mod. Phys.* **45** 574
Lemieux M A, Breton P and Tremblay A-M S 1985 *J. Physique Lett.* **46** L1
Levinshtein M E, Shklovskii B I, Sur M S and Efros A L 1976 *Sov. Phys.-JETP* **42** 197
Prunet V and Blanc R 1986 *J. Phys. A: Math. Gen.* **19** L1197
Sahimi M and Goddard J D 1985 *Phys. Rev.* B **32** 1869
Thorpe M F and Garboczi E 1987 *Phys. Rev.* B **35** 8579
Wang J 1988 *J. Phys. A: Math. Gen.* **21** L353
Zabolitzky J G, Bergman D J and Stauffer D 1986 *J. Stat. Phys.* **44** 211