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COMMENT

Re-examination of 3D percolation threshold estimates

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Abstract. Traditional Monte Carlo simulation of a $1000 \times 1000 \times 1000$ simple cubic lattice gave a bond percolation threshold near 0.2494 and a site percolation threshold near 0.3116 with probable error bars near 10^{-4}.

The Cray-2 vector computer has a main memory of 256 megawords, allowing simulations of very large systems. The Hoshen-Kopelman algorithm for percolation [1] can perhaps be vectorised for the simultaneous simulation of many lattices [2] but it is difficult to vectorise its recursive classification of clusters in one system. Thus employing a standard (i.e. not vectorised) program [3], for which the Cray-2 has about the same speed as the CDC Cyber 76, we utilised its large memory by simulating one lattice of linear dimension $L = 1000$. (Actually we used an older prototype of the Cray-2 with 'only' sixteen million memory words.) One sweep through the whole simple cubic lattice took about 3 h for bond and 1 h for site percolation.

We found the bond lattice to percolate at a concentration of 0.2495 but not 0.2494. The standard deviation for p_c is known to vary as $L^{-1/\nu} = L^{-1.14}$ and is about 0.000 62 for $L = 200$ (from reference [4]); thus it is about 0.000 10 for $L = 1000$. The shift due to finite-size effects is $0.07/L^{1/\nu} = 0.000\ 03$ for our system size, as found by comparison with $L = 65$ in reference [4] ('helical' boundary conditions). Our resulting threshold estimate 0.2494 also agrees well with the effective threshold 0.2495 ± 0.0001 found from eight independent runs for $L = 300$. Thus the present estimate $p_c = 0.2494$ has a probable error near 0.0001 and is compatible with Wilke's 0.2492 ± 0.0002. Presumably the truth is in between: $p_c = 0.2493$. Grassberger's [5] estimate 0.2488 is slightly lower. Since we used the same program as Wilke, the possibility of a programming error instead of an extrapolation error cannot thus be ruled out but is unlikely.

Site percolation is simpler but less controversial. Our $L = 1000$ lattice percolated at 0.3117 but not at 0.3116; comparison with $L = 100$ gave a downward shift $0.27/L^{1/\nu}$ which is about 0.0001 at $L = 1000$. Taking into account five runs at $L = 300$ with a rather high effective threshold 0.3122 ± 0.0003 we finally estimate $p_c = 0.3116 \pm 0.0002$, in excellent agreement with earlier slightly less accurate estimates [6] of 0.3117, 0.3118 and 0.3115.

Thus with the same technique and the same computational effort as on smaller computers we utilised the Cray-2 to get a more reliable result nearly free from finite-size errors. We confirmed that references [4, 6] made correct extrapolations for the finite-size effects.

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