Appendix

Throughout the guide we have encountered a number of algorithms. It was intended that everyone who actively participated in the guide would be able to try out the presented algorithms. All the algorithms given in the text were given in the pseudo-programming language. We realize that at the moment not everybody is familiar with an algorithmic language. A guide, however, is of no use when the participants cannot sit down and do the simulations by themselves.

To help to ease the conversion from the algorithmic language into FORTRAN we include in this appendix FORTRAN versions of two of the basic algorithms. The participant will by now have a feeling for how some of the problems are attacked and will find no difficulty in adapting the given FORTRAN programs to other algorithms given in the text.

A.1 Algorithm for the Random Walk Problem

The first listing is a program for the simple sampling of random walks.

```
c-------------------------------------------------------------c
c                           Algorithm                         c
c                                                             c
c          Simple Sampling for the Random Walk Problem        c
c                                                             c
c                       Dieter W. Heermann                    c
c                            Oct. 1987                        c
c-------------------------------------------------------------c

       integer nwalk,n,iseed,ip
       real    r,edx,edy,edxs,edys,xsqr,ysqr
c
c
       write(*,*) 'step length of walk'
       read(*,*) n
c
       write(*,*) 'how many walks'
       read(*,*) nwalk
c
```

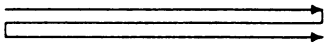
```
      write(*,*) 'seed '
      read(*,*) iseed
c
      edx = 0.0
      edy = 0.0
c
      edxs = 0.0
      edys = 0.0
c
      do  10  i=1,nwalk
        x = 0.0
        y = 0.0
c
        do  20  j=1,n
c
c           generate one step
            r = random(iseed)

            ip = r * 4
            if ( ip .eq. 0 ) x = x + 1.0
            if ( ip .eq. 1 ) y = y + 1.0
            if ( ip .eq. 2 ) x = x - 1.0
            if ( ip .eq. 3 ) y = y - 1.0

   20     continue
c
c       accumulate the result
        xsqr = x * x
        ysqr = y * y
c
        edx = edx + xsqr
        edy = edy + ysqr
c
        edxs = edxs + xsqr * xsqr
        edys = edys + ysqr * ysqr
c
   10   continue
c
c     perform the averaging
      edx = edx / float(nwalk)
      edy = edy / float(nwalk)
c
      write (*,*) edx, edy, edxs, edys
c
      stop
      end
```

A.2 Algorithm for Cluster Identification

The algorithm to identify all clusters in a given percolation configuration is based on an idea first proposed by *Hoshen* and *Kopelman* [A.1]. This idea was further

developed by *Kertesz* (J. Kertesz, Private communication) and the algorithm described below makes extensive use of his development.

The algorithm uses labels which we also found useful for other algorithms given in the text. Suppose we scan the lattice from the upper left corner to the upper right corner and continue with the next row starting from the first site of the left edge:



etc.

This is rather like a typewriter working its way across the paper. We start by labeling the first occupied site with a "1". If the next site is occupied we carry the label "1" to this site. If we find another occupied site which is not connected with the cluster labeled "1", we label it with a "2", etc. Assume we are somewhere in the lattice. All the sites above and to left have been worked on. Assume further that the current site is occupied. We check whether the site above the current site is occupied. If so we read the label of this site. Next we check whether the site to the left is occupied. If so, we read the label of this site. What label should be assigned? The labels of the site above and the site to the left might not be the same. The two sites can belong to two, until now, unconnected clusters. The current site is a link between them. Both clusters have different labels. We need a means of identifying different labels with each other.

The idea used to equate different labels is to use a sort of permutation vector. If the cluster labeled, say, "10" becomes a part of the cluster labeled "7" we make an entry in element number "10" that we should really look for label "7".

That two clusters have to be recognized as one cluster can, of course, occur more than once. The cluster labeled "7" may be connected to cluster "5". How do we identify the root label?

Each time two clusters are identified with each other the number of sites in the cluster increases by more than one unit. From where do we get the information on the number of sites in a cluster?

The two questions raised in the preceding paragraphs can be answered together. We introduce two kinds of pointers. Positive integer numbers signify the number of sites in the cluster. Negative integer numbers are the pointers to the next label. Going through the permutation vector we continue until a positive number is found.

A listing of a program where the idea outlined above is realized is given below.

```
c-------------------------------------------------------------c
c                            Algorithm                      c
c                                                           c
c          Simple Sampling of the 2D percolation Problem.   c
c                                                           c
c               Analysis of the droplet distribution.       c
c                                                           c
c                            Oct. 1987                      c
c                        Dieter W. Heermann                 c
c-------------------------------------------------------------c
c
      dimension lattice(20,20)
c
      dimension lptr(1000)
```

```
      dimension row(0:40)
      dimension vecl(1000)
c
      integer   lptr,row
      integer   up,left,cl
c
c
c     set the simulation parameters
c     -----------------------------
c
      write(*,*) 'linear lattice dim = '
      read(*,*) l
      write(**) 'give p='
      read(**) p
      write(*,*) 'give iseed         = '
      read(*,*) iseed
      write(*,*) 'give mcsmax        = '
      read(*,*) mcsmax
c
      write(9,*) 'simulation parameters are as follows'
      write(9,*) '====================================='
      write(9,*)
      write(9,*) 'perc 2d:   linear size = ',l
      write(9,*) 'iseed is                ',iseed
      write(9,*) 'mcsmax is               ',mcsmax
c
c     set up the random number generator
c     ----------------------------------
c
      iseed = iseed * 4 + 1
c
c
      maxi = 99999
      nsm  = 1000
c
c-------------------------------------------------------------------c
c                                                                   c
c      monte carlo part                                             c
c                                                                   c
c-------------------------------------------------------------------c
c
      do  200  mcs=1,mcsmax
       do   100  i=1,l
        do   100  j=1,l
          lattice(i,j) = 0
          if ( p .gt. ranf(iseed) )  lattice(i,j) = 1
 100   continue
c
c-------------------------------------------------------------------c
c                                                                   c
c      D r o p l e t  A n a l y s i s                               c
c                                                                   c
c      Dieter W. Heermann                                           c
c      October 1984                                                 c
c                                                                   c
c-------------------------------------------------------------------c
c
      cl = 0
      do  600  irow=0,l
         row( irow ) = maxi
 600   continue
c
      do  605  irow=1,l
c
       do  800  icol=1,l
c
         if (lattice(irow,icol) .eq. 1)                goto 805
           row(icol) = maxi
```

```
            goto 800
c
c         see if the spin is connected
c         ----------------------------
c
 805      up    = row( icol )
          left  = row( icol - 1)
c
          if ( up .eq. maxi )                                goto 815
          if ( lptr( up ) .gt. 0 )                           goto 815
            ms = lptr( up )
 810        la = - ms
            ms = lptr ( la )
            if( ms .lt. 0)                                   goto 810
              lptr( up ) = -la
              up         = la
c
 815      if ( left .eq. maxi )                              goto 825
          if ( lptr( left ) .gt. 0 )                         goto 825
            ms = lptr( left )
 820        la = -ms
            ms = lptr( la )
            if ( ms .lt. 0 )                                 goto 820
              lptr( left ) = -la
              left         = la
c
 825      mini = minO( up, left )
          if ( mini. ne. maxi )                              goto 830
c
c         spin is not connected. assign new label
c         ---------------------------------------
c
          cl                    = cl + 1
          row( icol )           = cl
          if ( cl .gt. nsm )                                    stop2
          lptr( cl ) = 1
          goto 800
c
c       spin is connected. find minimum label
c       -------------------------------------
c
 830    nofs = 1
        if ( up .eq. left )                                  goto 831
        if ( up .ne. maxi )  then
          nofs       = nofs + lptr( up )
          lptr( up ) = -mini
          end if
 831    if ( left .ne. maxi ) then
          nofs        = nofs + lptr(left)
          lptr( left )= -mini
          end if
        row( icol ) = mini
        lptr( mini ) = nofs
c
 800   continue
 605   continue
c
 200
       continue
c
       end
```

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See also [2.8, 2.10, 6.54, 6.61, 6.95]

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Appendix

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Bibliography

In the first five years after this book was first published (1987–1992) Monte Carlo (MC) computer simulation methods have been developed further in many respects. In the following some pertinent publications which complement the material of the present textbook are listed, in order to provide for the reader a first guide to the more advanced literature. Of course, only a limited, somewhat subjective selection can be given here.

Reduction of Slowing Down (Cluster algorithms, multigrid MC, etc.)

Edwards R.G., J. Goodman, A.D. Sokal: Multigrid MC: Two-dimensional XY model. Nucl. Phys. V **354**, 289 (1991)

Goodman J., A.D. Sokal: Multigrid MC for lattice field theory. Phys. Rev. Lett. **56**, 1015 (1986)

Goodman J., A.D. Sokal: Multigrid MC method: Conceptual foundations. Phys. Rev. D **40**, 2023 (1989)

Hasenbusch M., S. Meyer: Cluster update acceleration of interface roughening in the 3D Ising model. Phys. Rev. Lett. **66**, 530 (1991)

Janke W.: Test of single cluster update for the three-dimensinal XY model. Phys. Lett. A **148**, 306 (1990)

Kandel D., E. Domany, A. Brandt: Simulations without critical slowing down: Ising and three state Potts models. Phys. Rev. B **40**, 330 (1989)

Sokal A.D.: *Monte Carlo Methods in Statistical Mechanics: Foundations and New Algorithms* (Cours de Troisieme Cycle en Suisse Romande, Lausanne 1989)

Swendsen R.H., J.S. Wang: Nonuniversal critical dynamics in MC simulations. Phys. Rev. Lett. **58**, 86 (1987)

Swendsen R.H., J.S. Wang, A.M. Ferrenberg: 'New MC methods for improved efficiency of computer simulations in statistical mechanics': In *The Monte Carlo Method in Condensed Matter Physics,* ed. by K. Binder, Topics Appl. Phys., Vol. 71 (Springer, Berlin, Heidelberg 1992) Chap. 4

Wolff U.: Lattice field theory as percolation process. Phys. Rev. Lett. **60**, 1461 (1988)

Wolff U.: Collective MC updating for spin systems. Phys. Rev. Lett. **62**, 361 (1989)

Hybrid Monte Carlo / Molecular Dynamics, Fourier Acceleration, etc.

Batrounis G.G., G.R. Katz, A.S. Kornfeld, G.P. Lepage, B. Svetitsky, K.G. Wilson: Langevin simulations of lattics field theories. Phys. Rev. D **32**, 273 (1985)

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Mehlig B., D.W. Heermann, B.M. Forrest: Hybrid MC for condensed matter systems. Phys. Rev. B **45**, 679 (1992)

Histogram Analysis

Deutsch H.P.: Optimized analysis of the critical behavior in polymer mixtures from MC simulations. J. Stat. Phys. **67**, 1039 (1992)
Ferrenberg A.M., R.H. Swendsen: New MC technique for studying phase transitions. Phys. Rev. Lett. **61**, 2635 (1988)
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Binder K.: Phase transitions in reduced geometry. Ann. Rev. Phys. Chem. **43**, 33 (1992)
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Binder K., J.S. Wang: Finite size effects at critical points with anisotropic correlations: Phenomenological scaling theory and MC simulations. J. Stat. Phys. **55**, 87 (1989)
Borgs C., R. Kotecky: A rigorous theory of finite size scaling at first order phase transitions. J. Stat. Phys. **61**, 79 (1990)
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Applications

The applications of Monte Carlo methods are far too numerous to be listed here. Rather we refer the reader to some comprehensive books:

Binder K. (ed.): *The Monte Carlo Method in Condensed Matter Physics,* Topics Appl. Phys., Vol. 71 (Springer, Berlin, Heidelberg 1992)

Landau D.P., K.K. Mon, H.-B. Schüttler: *Computer Simulation Studies in Condensed-Matter Physics IV,* Springer Proc. Phys., Vol. 72 (Springer, Berlin, Heidelberg 1992)
Landau D.P., K.K. Mon, H.-B. Schüttler: *Computer Simulation Studies in Condensed-Matter Physics V,* Springer Proc. Phys., Vol. 75 (Springer, Berlin, Heidelberg 1993)

Subject Index