Applications of Monte-Carlo to Systems of Statistical Mechanics

System, many degrees of freedom, $(X) = (x_1, x_2, x_3, \ldots)$

Hamiltonian, $\mathcal{H}(X)$

$$Z = \int dX e^{-\beta \mathcal{H}(X)}$$

$$F = -k_B T \log Z$$

$$E = -\left(\frac{\partial F}{\partial T}\right)_V$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V$$

$$\ldots$$

Averages in the canonical ensemble:

$$\langle \mathcal{O} \rangle = Z^{-1} \int dX \mathcal{O}(X) e^{-\beta \mathcal{H}(X)}$$

$$E = \langle \mathcal{H} \rangle$$

$$C_V / k_B = \beta^2 \left[\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 \right]$$

$$\ldots$$

$$\langle \mathcal{O} \rangle = \int dX \mathcal{O}(X) f_{\hat{\mathbf{X}}}(X)$$

$$f_{\hat{\mathbf{X}}}(X) = Z^{-1} e^{-\beta \mathcal{H}(X)} = \frac{e^{-\beta \mathcal{H}(X)}}{\int dX e^{-\beta \mathcal{H}(X)}}$$

$$f_{\hat{\mathbf{X}}}(X) \geq 0$$

$$\int dX f_{\hat{\mathbf{X}}}(X) = 1$$

$$g(X|Y) h(X|Y) f_{\hat{\mathbf{X}}}(Y) = g(Y|X) h(Y|X) f_{\hat{\mathbf{X}}}(Y)$$

$$h(X|Y) = min(1, q(X|Y))$$

con

$$q(X|Y) = \frac{g(Y|X) f_{\hat{\mathbf{X}}}(X)}{g(X|Y) f_{\hat{\mathbf{X}}}(Y)}$$

Si $g(X|Y) = g(Y|X)$

$$h(X|Y) = min(1, e^{-\beta \Delta \mathcal{H}})$$

$$\Delta \mathcal{H} = \mathcal{H}(X) - \mathcal{H}(Y)$$

If $\Delta \mathcal{H} \leq 0$, accept.

If $\Delta \mathcal{H} > 0$, accept with probability $e^{-\beta \Delta \mathcal{H}}$

Glauber's choice

$$h(X|Y) = (1 + e^{\beta \Delta \mathcal{H}})^{-1}$$

Ising Model

Regular lattice in dimension d. Spin variable $S_i = \pm 1$.

$$\mathcal{H} = -J \sum_{<i,j>} S_i S_j - H \sum_i S_i$$

H is an external magnetic field

Coupling constant $J > 0$, ferromagnetic ground state

Critical temperature, T_c

Magnetization

$$m = \langle | \sum_{i=1}^{N} S_i | \rangle$$

Sample average:

$$m = \frac{1}{M} \sum_{k=1}^{M} m_k \pm \sigma_M$$

$m_k = |N^{-1} \Sigma_{i=1}^{N} S_i|$ Metropolis method, choose randomly a spin

$$X = s_1, s_2, \ldots, s_k, \ldots, s_N \qquad X' = s_1, s_2, \ldots, s'_k, \ldots, s_N$$

Only possible choice $s'_k = -s_k$.

Periodic boundary conditions

Neighbours table

$$n1(i),\ i=1,N \text{ East neighbour}$$

$$n2(i),\ i=1,N \text{ North neighbour}$$

$$n3(i),\ i=1,N \text{ West neighbour}$$

$$n4(i),\ i=1,N \text{ South neighbour}$$

Energy change:

$$\mathcal{H}_i = -Js_i \sum_{\mu} s_{i_\mu}$$

$$\mathcal{H}'_i = -Js'_i \sum_{\mu} s_{i_\mu} = +Js_i \sum_{\mu} s_{i_\mu}$$

$$\Delta\mathcal{H} = 2Js_i \sum_{\mu} s_{i_\mu}$$

$$-\beta\Delta\mathcal{H} = -2\beta Js_i \sum_{\mu} s_{i_\mu} \equiv -2KB_i = -2K \begin{cases} -4 \\ -2 \\ \ \ 0 \\ \ \ 2 \\ \ \ 4 \end{cases}$$

$$B_i = s_i \sum_{\mu} s_{i_\mu}$$

$$e^{-\beta\Delta\mathcal{H}} = e^{-2KB_i}$$

Keep in vector:

$$boltz(j) = e^{-2Kj}$$

```
      parameter (l=10,n=l*l)
      integer s(n)
      dimension n1(n),n2(n),n3(n),n4(n)
      dimension boltz(-4:4)
      real k
      data k /0.45/
      data mc /50/
      data m /100/
      do 100 i=1,l
      do 100 j=1,l
      ij=nij(i,j,0,0,l)
      n1(ij)=nij(i,j,1,0,l)
      n2(ij)=nij(i,j,0,1,l)
      n3(ij)=nij(i,j,-1,0,l)
      n4(ij)=nij(i,j,0,-1,l)
100   continue
      do 200 j=-4,4,2
      boltz(j)=exp(-2*k*j)
200   continue

      call dran_ini(12345)
      do i=1,n
      if (dran_u().lt.0.5d0) then
       s(i)=+1
      else
       s(i)=-1
      endif
      enddo

      rm=0.0
      rm2=0.0
```

```
      do 1000 im=1,m

      do 999 ij=1,mc*n
      i=i_dran(n)
      ib=s(i)*(s(n1(i))+s(n2(i))+s(n3(i))+s(n4(i)))
      if (dran_u().lt.boltz(ib)) s(i)=-s(i)
999   continue

      rm0=0.0
      do 20 i=1,n
      rm0=rm0+s(i)
20    continue
      rm0=abs(rm0/n)
      rm=rm+rm0
      rm2=rm2+rm0*rm0

1000  continue
      rm=rm/m
      rm2=sqrt((rm2/m-rm*rm)/m)
      write(6,*) rm,rm2
      end

      function nij(i,j,ix,jy,l)
      i1=i+ix
      if (i1.gt.l) i1=i1-l
      if (i1.lt.1) i1=i1+l
      j1=j+jy
      if (j1.gt.l) j1=j1-l
      if (j1.lt.1) j1=j1+l
      nij=(j1-1)*l+i1
      return
      end
```

Variations on a theme

Reduce calculation of random numbers

```
      if (ib.le.0) then
                       s(i)=-s(i)
      else if (ran_u().lt.boltz(ib)) s(i)=-s(i)
      endif
```

Sequencial updating

The N MC steps are performed sequentially:

```
      do 999 ij=1,mc
      do 999 i=1,n
      ib=s(i)*(s(n1(i))+s(n2(i))+s(n3(i))+s(n4(i)))
      if (ran_u().lt.boltz(ib)) s(i)=-s(i)
999   continue
```

Usefule for vector or parallel computers

Update sub-lattices

Systems with conserved order parameter

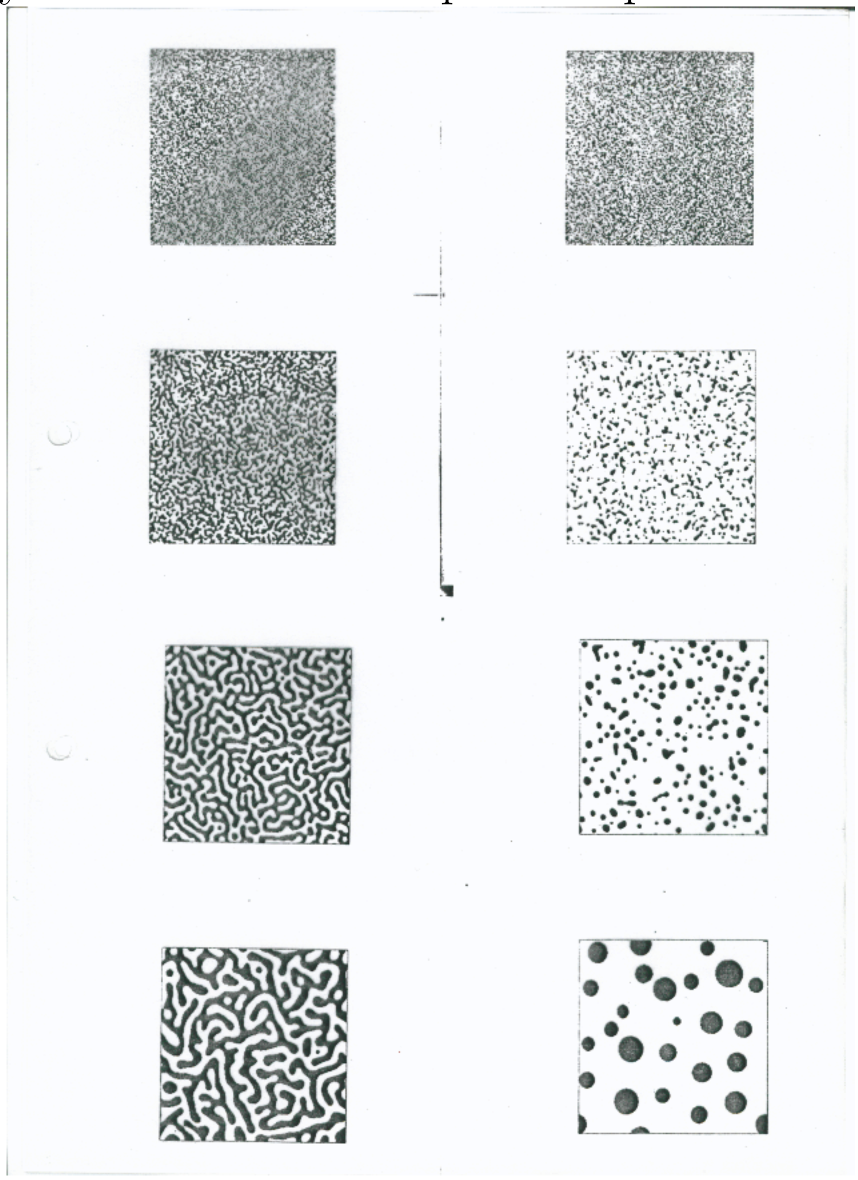
Kawasaki's proposal:

$$X = s_1, \dots, s_{k_1}, \dots, s_{k_2}, \dots, s_N$$

$$X' = s_1, \dots, s_{k_2}, \dots, s_{k_1}, \dots, s_N$$

Exchange of two next-nearest neighbour spins

Dynamical model for phase separation in binary alloys



Heat bath method

N-dimensional r.v. $\hat{\mathbf{x}}$, $(s_1, s_2, \ldots, s_N)$.

Proposal: change to: $\hat{\mathbf{x}}' = (s_1', s_2', \ldots, s_N')$ by changing only one variable:

$$f(x'|x) = f(s_i'|s_i)$$

Detailed Balance:

$$g(s_i'|s_i)h(s_i'|s_i)f_{\hat{\mathbf{x}}}(s_1, \ldots, s_i, \ldots, s_N) =$$

$$g(s_i|s_i')h(s_i'|s_i)f_{\hat{\mathbf{x}}}(s_1, \ldots, s_i', \ldots, s_N)$$

Solution:

$$g(s_i'|s_i) = g(s_i') = f(s_i'|s_1, \ldots, s_{i-1}, s_{i+1}, \ldots, s_N)$$

$$h(s_i|s_i') = 1$$

i.e, sample s_i' from a distribution in which the remaining variables are fixed. The new value for s_i' is independent from old value and always accepted. Remaining variables act as a heat bath.

Ising model

Heat bath Choose i. Choose s'_i with probability proportional to

$$f(s'_i|s_1 \dots s_N) \sim e^{\beta J s'_i \sum_{\mu=1}^{2d} s_i} \equiv e^{a_i s'_i}$$

where we have defined:

$$a_i = \beta J \sum_{\mu=1}^{2d} s_i$$

There are just two possible values

$$P(s'_i = +1) = \frac{e^{a_i}}{e^{a_i} + e^{-a_i}} = (1 + e^{-2a_i})^{-1}$$

$$P(s'_i = -1) = \frac{e^{-a_i}}{e^{a_i} + e^{-a_i}} = \frac{e^{-2a_i}}{1 + e^{-2a_i}}$$

```
      do 10 j=-4,4,2
      boltz(j)=1./(1.+exp(-4.*k*j)
10    continue
      do 100 ij=1,mc*n
      i=i_ran(n)
      j=s(n1(i))+s(n2(i))+s(n3(i))+s(n4(i))
      if (ran_u().lt.boltz(j)) then
                                s(i)
      else
                                s(i)=-1
      endif
```

Heisenberg model

Regular lattice in dimension d. Variable $\vec{S}_i$, con $|\vec{S}_i| = 1$

$$\mathcal{H} = -J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$

$$\mathcal{H}_i = -J \vec{S}_i \sum_{\mu} \cdot \vec{S}_{i_\mu}$$

$$e^{-\beta \mathcal{H}_i} = e^{\vec{S}_i \cdot (K \sum_\mu \vec{S}_{i_\mu})} \equiv e^{\vec{S}_i \cdot \vec{H}_i} = e^{H \xi_i}$$

with $\xi_i = \cos(\theta_i)$, angle between local field $\vec{H}_i$ and variable $\vec{S}_i$.

$$\vec{S}_i = (\phi_i, \theta_i) = (\phi_i, \xi_i)$$

$$g(\vec{S}_i) = g(\phi_i) g(\xi_i)$$

$$g(\phi_i) = (2\pi)^{-1}, \text{ si } \phi_i \in (0, 2\pi)$$

$$g(\xi_i) = C e^{H_i \xi_i}$$

Exponential distribution:

$$\begin{aligned} \xi_i &= \frac{1}{H_i} \ln \left(1 + \hat{\mathbf{u}} (e^{2H_i} - 1) \right) - 1 \\ \theta_i &= \arg\cos(\xi_i) \end{aligned}$$