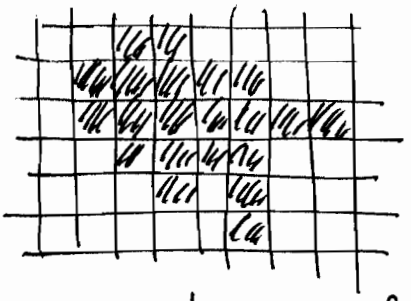
CLUSTER MOVES (§14.3 in F+S)

Systems which naturally form clusters of particles can pose problems in simulations -

e.g. * systems near critical points

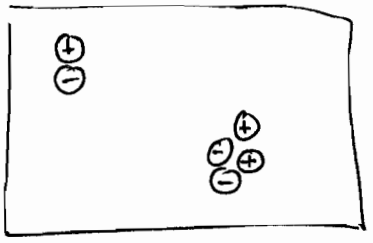


Spin ↑ or occupied

Spin ↓ or unoccupied

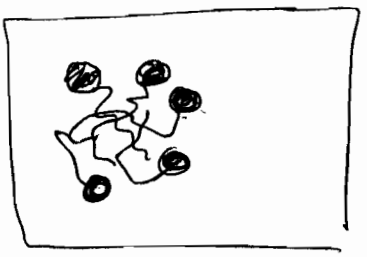
For a grand canonical simulation of such a system, it is difficult to create a single hole in the middle of a cluster of occupied sites - system evolves slowly through configuration space

* systems with very strong interactions - e.g. associating or ionic systems



For temperatures relevant for phase separation, interaction energy between opposite-charge particles is $\sim 20\,kT$, so pairs stay "bound" - again, it is difficult to sample configuration space

* Systems that aggregate - e.g. amphiphile solutions forming micelles



↑ head - hydrophilic

↑ tail - hydrophobic

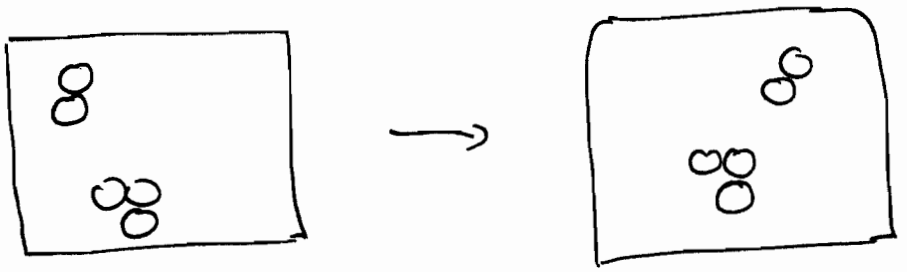
Simple version of cluster moves

Wu, Chandler, Smit J. P. C. 96, 4077 (1992).

Define a criterion for cluster formation:

→ if two particles are less than a certain distance r_c, then they belong to the same cluster

Perform a move in which a complete cluster is displaced:



Check if any new clusters are formed in the new configuration: if yes, reject move.

If this is not done, detailed balance is violated: new clusters are formed, but cannot break up.

If no new clusters are formed, accept/reject with Metropolis criterion $P_{acc} = \min\left[1, \exp(-\beta \Delta U)\right]$

Probabilistic bond formation

A generalization of the previous approach is one in which two particles k, ℓ form a "bond" (belong to the same cluster) with probability $P(k,\ell)$ that depends on their distance (or energy of interaction or relative orientation)

Detailed balance requires that:

$$\left\{\begin{array}{l}\text{Probability of finding system}\\ \text{in "old" state}\end{array}\right\} \times \left\{\begin{array}{l}\text{Probability of forming}\\ \text{a specific cluster}\\ \text{in "old" state}\end{array}\right\} \times P_{acc}(o \to n)$$

$$= \left\{\begin{array}{l}\text{Probability of finding system}\\ \text{in "new" state}\end{array}\right\} \times \left\{\begin{array}{l}\text{Prob. of forming}\\ \text{the same cluster in}\\ \text{"new" state}\end{array}\right\} \times P_{acc}(n \to o)$$

$$\Rightarrow \exp(-\beta U_o) \cdot \prod_{ke} \left(1 - p^{old}(k,e)\right) \cdot P_{acc}(o \to n) =$$

$$= \exp(-\beta U_n) \cdot \prod_{ke} \left(1 - p^{new}(k,e)\right) P_{acc}(n \to o)$$

→ k denotes a particle in the cluster and l one outside it. ←

Note that the probability of forming a specific cluster in the old or new states is

$$\underbrace{\left(\prod_{k,k'} p(k,k')\right)}_{\text{this term does not change during a cluster move, since the relative distances of the particles in the cluster do not change.}} \cdot \left(\prod_{k,e} \left(1 - p(k,e)\right)\right)$$

Final result:

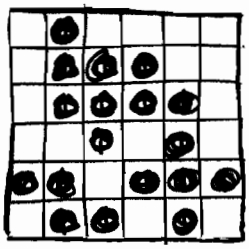
$$\frac{P_{acc}(o \to n)}{P_{acc}(n \to o)} = \exp\left(-\beta \Delta U\right) \cdot \prod_{ke} \frac{1 - p^{new}(k,l)}{1 - p^{old}(k,e)}$$

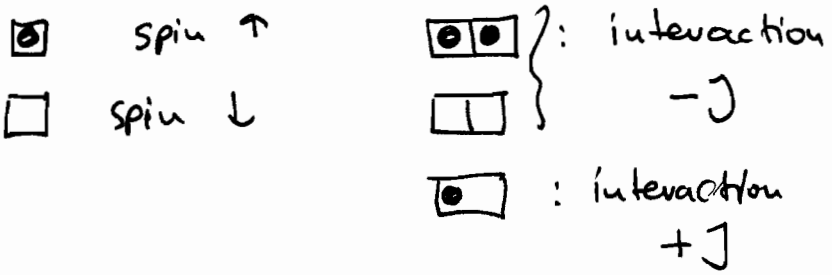
The simple case of cluster moves corresponds to the choice $p(k,e) = 1$ if $r_{ke} < r_c$.

[This scheme can be used for "early rejection" of moves that result in a high energy of interaction between two particles in a "normal" simulation]

Swedsen-Wang Algorithm PRL 58, 86 (1987)

Swedsen + Wang proposed a scheme to eliminate critical slowing-down in Ising simulations.



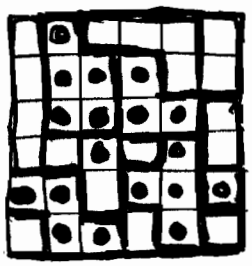


Consider a configuration with N_a antiparallel spin pairs, N_p parallel spin pairs

$$U = (N_a - N_p) \cdot J$$

Generate clusters according to the following rules:

- If nearest neighbors antiparallel, not connected
- If nearest neighbors parallel, connect w/ prob. p

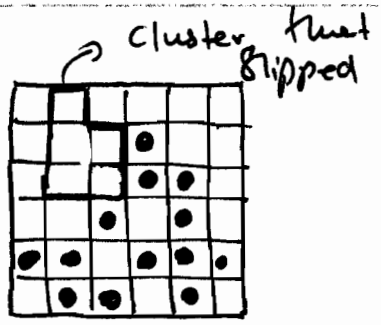


← heavy lines indicate one possible partitioning into clusters. The probability of n_c parallel spins being connected in a specified arrangement is

$$p^{n_c} \cdot (1-p)^{N_p - n_c}$$

Now, select a cluster to "flip" — all particles change spin, "Δ" change in parallel spins:

$$N_p(\text{new}) = N_p(\text{old}) + \Delta \qquad N_a(\text{new}) = N_a(\text{old}) - \Delta$$



($\Delta = +2$ in this case)

$$u(\text{new}) - u(\text{old}) = -2J\Delta$$

Probability of reverse move: Construct same cluster structure, but from $N_p + \Delta$ ↑↑ spinpairs and $N_a - \Delta$ ↑↓ spin pairs

Connected bonds do not change; However, there are now $(N_p + \Delta)$ parallel spin pairs, so that the probability is $p^{n_c} \cdot (1-p)^{N_p + \Delta - n_c}$

Detailed balance condition:

$$\exp(-\beta u_{old}) \cdot p^{n_c} \cdot (1-p)^{N_p - n_c} \cdot Acc(old \to new) =$$

$$= \exp(-\beta u_{new}) \cdot p^{n_c} \cdot (1-p)^{N_p + \Delta - n_c} \cdot Acc(new \to old)$$

$$\Rightarrow \exp(-2\beta J\Delta) = (1-p)^{\Delta} \cdot \frac{Acc(new \to old)}{Acc(old \to new)}$$

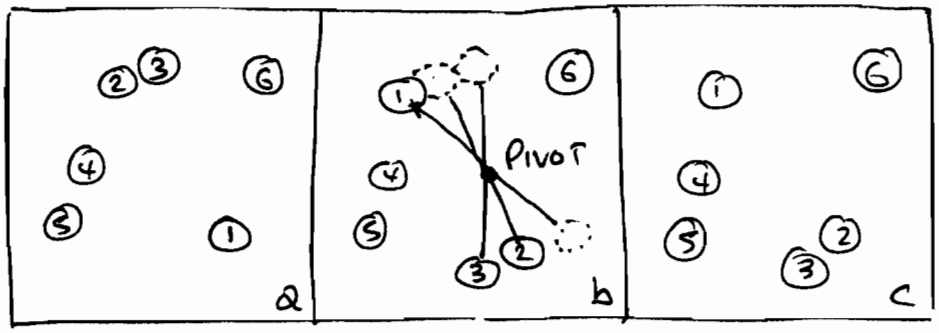
We can have $Acc(new \to old) = 1$ by setting

$$\exp(-2\beta J) = 1 - p \Rightarrow \boxed{p = 1 - \exp(-2\beta J)}$$

SW "dynamics" are extremely fast!

Geometric Cluster Algorithms

See Liu + Luijten, Phys. Rev. Lett. 92:035504 (2004)



* pick random "pivot" point
* Select random particle to reflect w.r.t. pivot
* If this leads to overlaps, move particles by reflection w.r.t. pivot until no more overlaps are present

For general potentials, particles are identified that interact with the moved particles and added to the cluster that moves with probability

$$P = \max\left[1 - \exp(-\beta \Delta_{ij}), 0\right]$$

where $\Delta_{ij} = \left| V(|r_i' - r_j|) - V(|r_i - r_j|) \right|$

r_i': new position of i; r_i: old position of i

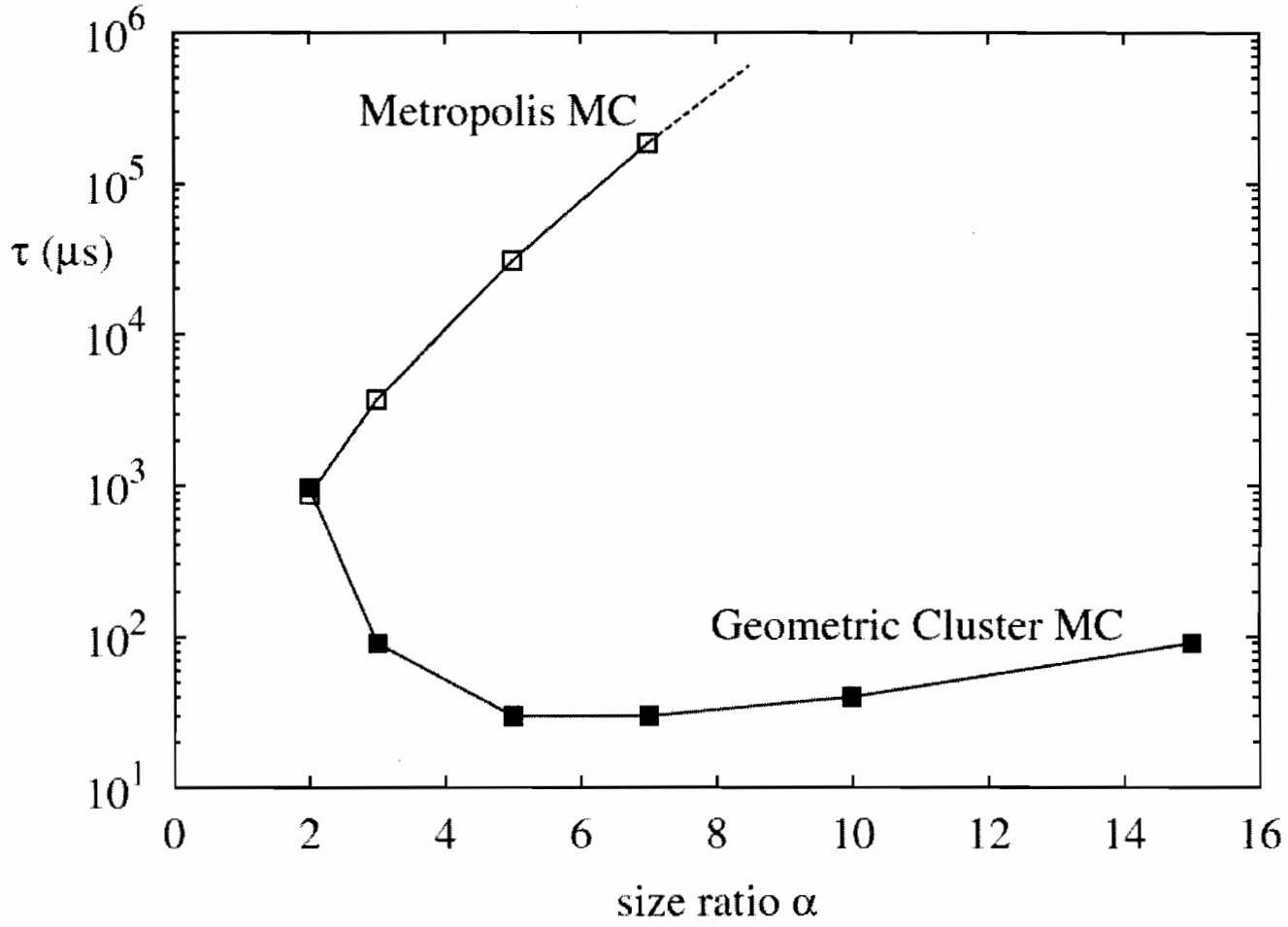


FIG. 3. Efficiency comparison between a conventional local update algorithm (open symbols) and the generalized geometric cluster algorithm (solid symbols), for a size-asymmetric binary mixture of Yukawa particles. As opposed to the local algorithm, the autocorrelation time per particle (expressed in microseconds of CPU time) for the GCA depends only weakly on size ratio α (variations correspond to changes in the volume ratio of large vs small particles in the cluster), resulting in an efficiency improvement of several orders of magnitude already for moderate α.