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Modelling frustration for physical systems

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MODELLING FRUSTRATION FOR PHYSICAL SYSTEMS

A Thesis

Presented to

**The Faculty of the Department of Physics
San Jose State University**

In Partial Fulfillment

**of the Requirements for the Degree
Master of Science**

By

Ines Mariana Suarez

May 1990

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This thesis is dedicated to my parents, Marilu and Carlos Suarez, for their continuing support and encouragement throughout my education, and to my husband, Kevin Barnes, for making all tough times easier to handle.

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ABSTRACT

MODELLING FRUSTRATION FOR PHYSICAL SYSTEMS

by Ines Mariana Suarez

Frustration is essential in understanding the basics of dynamics and statics in structural glasses, spin-glasses, neural networks, and other frustrated systems. To describe this major concept, computational studies were performed using a simple frustration model. This frustration model is similar to but more general than the Ising model. Results including clustering effects are presented and discussed in detail. In this work, pattern formation, and periodic and apparently random motion have been observed. Temperature dependence studies are included. Indications of the existence of a critical temperature have been found, as well as precursor effects signaling the onset of the freezing process. Based upon this tentative success, plausible applications of this frustration model are presented. In particular, a discussion of possible applications to systems such as (spin) glasses is included.

INTRODUCTION FOR NON EXPERTS

This thesis introduces a new computational model to study the effects of frustration in physical systems. The results obtained with this model are included. The concept of physical frustration is very similar to the concept of frustration in social science.

When two or more interacting characters (let it be persons, particles, spins, etc.) have opposing needs, each character will pull toward the direction which will satisfy its own needs. This creates a frustrating situation between the characters which cannot always be resolved. Most likely, the characters will try to select between the many possible solutions for the solution which creates the least tension or frustration between them. However, the "best" possible solution may not always be at hand, and the characters will have to opt for a "better" solution. The interaction between characters can be represented by a set of values (matrix) which determines how strong or weak the interactions are.

The possible solutions constitute a set which may include a great number of solutions. The situations included in such a set are all different and therefore some are "better" than others. Some of these solutions are more likely to be chosen than others; such are called stable solutions. Some solutions are very unlikely to be chosen; such solutions are called non-stable solutions. Somewhere in between stable and non-stable solutions, there exist some solutions that are likely to be chosen, but are not

completely stable; such solutions are called metastable solutions. The set can be visualized as a mountainous landscape. The valleys in such a landscape would be the stable solutions and the hills would be the non-stable solutions. Sometimes a valley from one perspective could be also a hill from another perspective. This could happen in the passage between two valleys which is surrounded by mountains, i.e., a saddlepoint. Such a situation corresponds to a metastable solution. This mountainous landscape represents the frustration state space. Therefore, it is said that the frustration state space possesses multivalley features, and this is actually a direct consequence of frustration.

The algorithm used for the frustration model presented in this thesis is fairly simple and uses several well-known computational techniques. The algorithm will be described in detail and the results obtained will be presented. These results include the fact that the model actually creates a frustration state space with a multivalley structure.

When the set of characters, which will be called a system, moves towards minimizing its frustration (i.e., when the system searches for a valley), the configuration of such system changes as well. The system as a whole can be observed as a point moving in between the mountains and valleys. The value for the frustration of the total system in such point can be viewed as the height of that point. How fast the system moves in this landscape toward finding a valley or "equilibrium" state, indicates the relaxation in time. The point representing the system can be compared with a

ball rolling on a rough uneven surface. At first it might happen that the ball has enough energy to roll around valleys at a fairly fast rate without stopping in them. However, sooner or later the ball will lose its energy and "get stuck" in one of the valleys, unable to jump the surrounding hills (barriers), and eventually stop at the base of one of the valleys.

When the temperature of the system is increased, the energy of the system is increased. If this happens, the system will take more time to relax to an "equilibrium" position. Eventually, if the temperature of the system is high enough, the system may never stop, or may take an extremely long time compared to the time one is willing to spend observing the system relax, which could easily be as long as the life of the universe. This would indicate that for a certain temperature, called critical temperature, the system would change its behavior drastically. Below the critical temperature, the system will eventually find an "equilibrium" position in a reasonable amount of time. Above the critical temperature, the system does not find an equilibrium position, or the amount of time that would take the system to find a valley is unreasonable.

Temperature dependence studies applying the frustration model were analyzed. A critical temperature and therefore a phase transition was found. This critical temperature depends on the number of characters in the system and the type of interaction between the characters.

Glass is both one of the oldest and newest materials. Despite 4000 years of experience and recent novel research, no reasonable foundation for the science of glass has been developed [4]. Several fundamental questions need to be addressed. The model of frustration described in the thesis may be successfully applied to various kinds of systems including the ones studied by the physics of disordered matter, such as (spin) glasses, which have raised a number of controversies in the last decades. Such systems will be addressed in the thesis.

CHAPTER 1

INTRODUCTION AND BACKGROUND.

FRUSTRATION

Frustration is a unique and relatively new physical concept, essential in the description and understanding of several disordered natural systems [1]. Such systems become frustrated when conflicting requirements imposed on different elements of a system compete in pursuit of the best compromise. Degeneracy in a system is found by measuring the minimum of a system parameter such as energy in the presence of these conditions. The frustration of a system is a measure of its degeneracy. As the degeneracy of a system increases, the number of possible configurations for approximately the same minimum energy increases as well.

If a system is both frustrated and disordered, it no longer possesses a unique ground state -- the system has a quasi-degenerate ground state. The energy surface presents a multivalley structure, which forms a mountainous landscape in state space. By understanding the effects of frustration and disorder with a relatively simple model, we may understand the way more complex frustrated systems behave.

Understanding more about the details of frustration will help us develop the physical concepts of disordered systems. With this goal in mind, the aim of this research is to study a relatively simple frustration model expanded using computational techniques.

A brief description of some relatively well-known frustrated systems will follow, in particular a short introduction to spin glasses and neural networks.

RANDOM DISORDERED AND FRUSTRATED SYSTEMS.

In general, physical theories derived to describe real materials use simplifications; for example, they often consider such materials as idealized pure systems. However, crystals invariably contain defects and impurities. Liquids invariably have impurities dissolved in them. The effects of these defects and impurities and to what extent the physical theories should be changed when describing real materials are the main concerns of the theory of disordered matter [2].

Many natural complex systems, including structural glasses [4], spin-glasses [1,3], proteins [5], and neural networks [6], have features in common arising from disorder, nonperiodicity, and frustration.

From a statistical point of view, disorder is often classified as quenched or annealed. Quenched disorder exists when the defects

or impurities, which are randomly distributed, do not equilibrate in the temperature range in which the properties of the system are changing. This equilibration can be a very slow process, often involving time constants which are comparable to the age of the universe. Annealed disorder is the opposite case, when the disorder distribution is changing in the temperature range of interest.

The effects of disorder begin at the microscopic level [2]. Amorphous solids and spin glasses are disordered in spatial and directional orientation, respectively. Proteins are also disordered, if we take into account their non-symmetry and non-periodicity in space.

Because all the competing requirements imposed on different elements of a system cannot be satisfied, the system becomes frustrated. In glasses, frustration arises intrinsically from variations in interatomic forces and randomness. The magnetic moments in spin glasses owe their dynamics and complexity to conflicting magnetic interactions. In these materials, ferromagnetic and antiferromagnetic interactions compete against each other. Proteins can be frustrated in the sense that a particular amino acid residue has multiple interactions with neighboring atomic complexes and may have two or more favored states resulting from these interactions.

Randomness also manifests its effects on the critical behavior of a system. One of the most important questions arising from these effects is whether or not the phase transition occurs at a

unique critical temperature T_c or if such transition is smeared out over some temperature interval.

Glasses are obtained by continuously supercooling the liquid state, that is, without undergoing the first order transition found in the formation of crystals. Theory has been difficult to formulate, in part because glass is not in thermal equilibrium and the atomic glass structure is not periodic. The microscopic structure of glass is not clearly understood and there are currently two different views to describe such structure:

- glasses, although non-crystalline, are continuous on an atomic scale;
- glasses form clusters that are weakly interconnected [4].

In spin-glass studies, opposing views are also presented [1,3]: the homogeneous spin-freezing process conflicts with spin-clustering effects observed near and below the spin-glass temperature. The following section focuses on (spin) glasses and neural networks.

SPIN GLASSES AND NEURAL NETWORKS

Spin glasses [7,8] are random magnetic systems, which, due to some structural disorder, have magnetic moments with competing interactions. These materials exhibit a transition for a given "freezing" temperature called the spin-glass temperature T_g , under which the spins actually "freeze" aligning in random

directions. The random freezing of the localized spins occurs in a cooperative manner. This leads to unusual properties which in many ways resemble a glass. For example, in the magnetic responses, a number of irreversibilities, metastabilities, and time dependencies appear. Below T_g , the highly irreversible, metastable frozen state occurs without the usual long-range spatial order [1,2,3]. Only phenomenological and partially successful theories for the (spin) glass transition exist.

Some of the properties that spin-glass systems possess are:

- a peak in the frequency-dependent susceptibility, due to the frozen-in magnetic moments below T_g ;
- a magnetic specific heat, linear in temperature;
- a lack of long-range magnetic order;
- when the magnetic field changes, there is remanence and magnetic relaxation on macroscopic time scales below T_g [7].

Competing exchange interactions and randomness yield the fundamental ingredient of a spin glass, frustration. One well known experimental result of spin-glass frustration is that many possibly unrelated low-energy states occur near and below T_g . The frustration ground state is multidegenerate; i.e., there exist many local energy minima in phase space very close in energy to the actual ground state.

One of the key questions in spin-glass science is how the spin system enters the glassy state. The frustration model presented in the next chapter may be successfully applied to this freezing

process, and perhaps in future may be used to attempt to solve the controversies in glass and spin-glass research.

Neural networks are large and highly interconnected assemblies of simple elements called neurons. The neurons are usually two-state devices. When their input exceeds a specific "firing" threshold value, they switch from one state to the other. Physicists became interested in such networks due to the analogy between these networks and magnetic systems [6,9]. In particular, there is an equivalence between the long-time behavior of networks with symmetric connections and the equilibrium properties of magnetic systems such as spin glasses. Long-range spin glasses and neural systems have many features in common:

- - the spatial configuration in both systems presents no resemblance to the crystalline order of pure magnets or solids;
- - the spin or neuron couplings in spin glasses or neural networks can be positive or negative;
- - each spin or neuron is connected with many others.

However, long-range spin glasses and neural systems possess differences as well:

- - the connections in neural systems are not distributed at random as in the case for spin glasses, but rather, the correlations are formed both genetically and in the process of learning;

-- the pairwise interactions between neurons are not in general reciprocally symmetric, which may make the dynamical properties of a neural system very different from those of equilibrium magnetic systems in which the pairwise interactions are reciprocally symmetric.

CHAPTER 2

MODELS

INTRODUCTION

This chapter and the one following contain descriptions of a proposed frustration model, and many of the results obtained with it.

A short introduction to the two-dimensional Ising model will be presented. The Gold model from which the idea of a frustration model originated will be described briefly, and essential modifications made in order to address physical concepts will be discussed. A complete account of the frustration model itself and a comparison with the Ising model will also be given. The different versions of the model studied and the main results obtained will be presented in Chapter 3.

ISING MODEL IN TWO DIMENSIONS

One of the simplest magnetic models is the Ising model. This model was first introduced as an attempt to simulate ferromagnetic materials. The one- and two-dimensional Ising models can be solved exactly using statistical methods. The two-

dimensional Ising model yields a nontrivial example of a phase transition.

The Ising model consists of an array of N fixed lattice sites which form an n -dimensional periodic lattice [10]. Such a lattice can have a geometrical structure which can be cubic, hexagonal, etc. Each of the N fixed points have an associated variable S_i , where $i=1,\dots,N$. Each of these spin variables can take on a value of $+1$ or -1 , which determines if the spin at each site is up ($+1$) or down (-1). A certain configuration of the system is specified by a given set of values $\{S_i\}$. The Hamiltonian of the system in the configuration specified by $\{S_i\}$ is:

$$H = - \sum J_{ij} S_i S_j - h \sum S_i$$

where the first sum is a double sum over $\langle ij \rangle$, which denotes a nearest neighbor pair of spins (each character possesses a total of four nearest neighbors). The second sum is over all spins i . Note that H is invariant when i and j are exchanged. J_{ij} is the exchange interaction between spins and h is the external magnetic field.

In a pure Ising ferromagnet [9], all the J_{ij} 's have the same value $J>0$; that is, pairwise interactions between two spins tend to point them in the same direction. ($J<0$ corresponds to an antiferromagnet, i.e., spins tend to point in opposite directions).

A pure Ising ferromagnet has two phases:

-- at temperatures large compared with J , the entropy dominates the energy and the spins fluctuate in an almost independent

fashion. Here the spontaneous magnetization $m = \langle S_i \rangle$ is zero, where the brackets mean an average over a very long time; -- at temperatures small compared with J , the energy dominates the entropy and the spins are all aligned in the same direction. There are, therefore, two equilibrium states which are equivalent (up or down). When the system chooses between the two states, the symmetry is said to be broken and $m = \langle S_i \rangle$, the spontaneous magnetization, is non-zero.

The transition between the two phases occurs at a critical temperature T_c which is different than zero only for $n > 1$. For $n > 1$, T_c is of the order of J .

GOLD MODEL

The attempt to understand the properties of frustration began with a model created by Richard Goldstein (Rich Gold) [11] and described in detail by A.K. Dewdney [12]. The Gold model consists of N characters able to move about a finite two-dimensional square lattice in which M non-mobile characters are present. Each character has an assigned ideal preferred distance I_{ij} with respect to all other $(N-1)+M$ characters, representing each character's repulsion or attraction for the others. The N characters start from assigned or random positions and are allowed to relax to a minimum in their total "unhappiness" given by the equation

$$U_i = \sum |D_{ij} - I_{ij}| ,$$

where the sum is over j, and D_{ij} is the actual distance between characters.

Each mobile character moves in turn to the one neighboring position (of a total of eight) which will give the lowest unhappiness. If none of the new positions of a character will lower the unhappiness, the character will remain in the original position. This makes the algorithm have the connotations of a steepest descent method [13].

FRUSTRATION MODEL

As mentioned by A. K. Dewdney [12], the notion of an ideal distance is used by behavioral scientists. This "social distance" is studied by proxemics. By coding the distances that people naturally tend to adopt in relation to others, "one can determine possible outcomes of the mix in terms of social dynamics" [12]. Along similar lines, the idea came up of using a similar model to mimic physical systems. The Gold model appeared to be an effective way to describe frustration in physical systems. In order to adapt this model to meet the needs of the research, it was necessary to assign physical meaning to the model. A cost function called "total frustration" was defined by the equation:

$$F = \sum (D_{ij} - I_{ij})^2,$$

where the sum is a double sum over all characters (i and j).

Again, D_{ij} is the actual distance between characters i and j, and I_{ij} is the i,jth element of the ideal distance matrix, representing the ideal distance character i desires to keep with respect to character j. This matrix is fundamental in the model. Its elements I_{ij} are set at the beginning of the program. They can be chosen at random or defined such that they describe a predetermined structure. Choosing these elements is the main way through which frustration is incorporated into the system. Note that I_{ij} may be different from I_{ji} , i.e., asymmetric pairwise interactions. See Appendix A for more detail.

The characters move to minimize their own individual frustration given by

$$F_i = \sum (D_{ij} - I_{ij})^2,$$

where the sum is a single sum over all characters j. This actually allows the total frustration to increase, since at each time step, an individual character's move is independent of the rest. Therefore, a character's move towards its minimum frustration may cause one or more characters to raise their individual frustration, which in turn may cause the whole system's frustration to increase.

The characters will move until they reach an "equilibrium" for the system, relaxing to the configuration which will determine the total minimum frustration.

The room may be allowed to take on different boundaries, including infinite boundaries. Infinite boundaries deserve special attention since they allow observation of the dynamic properties of the system. Most of the major findings of this thesis have been obtained using infinite boundaries. Infinite boundaries are not as deceptive as fixed boundaries which can cause the characters to "bounce" against the walls, or periodic boundary conditions which can distort the presence of clustering formation, or falsely enhance cluster formation.

The first attempts to describe frustration modifying Gold's model, were using the following tentative algorithm:

- choose initial positions at random;
- set ideal distance matrix;
- select a character and compute its frustration;
- check the frustration this character will have if moving to any of the eight neighboring positions;
- move character to the position which gives the lowest frustration, unless that position has been already occupied by another character;
- select another character and start process again;
- once all characters have been moved (one iteration or time step) calculate the total frustration for the whole system;

- - repeat this process until the system comes to a fairly stable configuration, that is, when the total frustration reaches a stable minimum.

This algorithm will be referred to in the following discussions as Algorithm 1. Some of the results obtained with this algorithm will be presented in Chapter 3. Note that Algorithm 1 does not include temperature; the absolute temperature is considered to be zero.

TEMPERATURE DEPENDENT FRUSTRATION MODEL

In order to consider possible phase transitions and subsequent application of critical phenomena theory, a set of steps that would include temperature dependence in the algorithm needed to be included. A temperature distribution of the Boltzmann type was used in the well-known Metropolis algorithm [14] and incorporated in the above described algorithm.

At each time step, the characters are allowed to randomly choose a move in a Moore Neighborhood; i.e., the characters randomly select any of their eight neighboring spaces, or they remain in their original position. Unlike in the case of Algorithm 1 where a character checks out all eight neighbors, after randomly selecting a neighboring space, the character compares its frustration in the selected space with the space it is presently occupying. The character will therefore move to the new position

or stay in the old one according to the criterion used in the algorithm described below. This change seems to give a slight difference in the relaxation rate of the system as will be shown in the next chapter. Again multiple occupation of sites is forbidden. Algorithm 1 and its changes constitute Algorithm 2. The results of the latter will also be presented in Chapter 3.

The following Monte Carlo type algorithm was used in Algorithm 2:

```
-- choose a character at random;
-- choose one of the eight neighboring spaces at random;
-- calculate the new individual frustration ( $F_{new_i}$ );
-- calculate the difference in frustration between the potential
   new position and the old one:  $\Delta F_i = F_{new_i} - F_i$ ;
-- if  $\Delta F_i < 0$  move character to new position;
-- if  $\Delta F_i > 0$  then: if  $p = \exp(-\Delta F_i/T) < TOL$  (  $TOL$  is a random
   number between 0 and 1) then stay in old position, else move
   to new position.
```

One iteration or time step is completed when all N mobile characters have been moved in this manner.

The case where $T=0$ deserves special care. The last two steps in the algorithm in this case reduce to:

```
-- if  $\Delta F_i < 0$  then  $p=1$ , therefore move to new position;
-- if  $\Delta F_i > 0$  then  $p=0$ , therefore stay in old position.
```

One computational disadvantage of these models is that they are long-range interaction type models; thus, an update of all the positions of the N mobile characters is necessary, making the

computation very time consuming when N is large. Both algorithms in essence reflect the same frustration model.

A Fortran program of Algorithm 2 with no fixed characters and no boundaries is presented in Appendix B. Notice that the I_{ij} 's are taken to be all equal to a constant D. This can be easily changed to reflect different cases.

In order to consider whether or not this frustration model generates a phase transition, the behavior of certain quantities with respect to temperature should be studied. Two of the plausible quantities that could be analyzed are the average of total frustration after the initial exponential relaxation $\langle F \rangle$ and the variation or standard deviation of $\langle F \rangle$: $\Delta = \langle (F - \langle F \rangle)^2 \rangle$.

These two quantities are defined as follows:

$$\langle F \rangle = \frac{1}{(m - m_{\min})} \sum F(it),$$

summed over "it," which represents the current iteration or time step. $F(it)$ is the total frustration of the system at iteration "it." The quantity "m" is the total number of iterations taken before stopping calculations for a given temperature. The quantity "mmin" is the time step at which the average is desired to start upon initial relaxation; i.e., when the system is close to the final (minimum) configuration.

As described above, $\Delta = \langle (F - \langle F \rangle)^2 \rangle$, where the average is taken in the same way as for $\langle F \rangle$. However, for computational purposes, a property of the standard deviation, namely

$$\Delta = \langle F^2 \rangle - \langle F \rangle^2$$

needs to be used.

A Fortran program for the frustration model which includes these calculations as well as a temperature changing loop is attached in Appendix C.

COMPARISON WITH ISING MODEL

Neural networks have been modelled in their simplest form by the Hopfield model [6]. The model, in general, consists of a set of variables S_i which can take on values ± 1 . S_i represents a neural cell as a two state device; its value is +1 when the cell is fired due to a given threshold voltage, -1 when it is not. In the case of spin glasses for example, S_i represents a spin up or down. In any frustrated system, S_i is a switch that will make an element of the system operative or not.

The magnetic exchange interaction J_{ij} , or the strength of the synapse between neural cells, is an essential parameter in the total Hamiltonian for a magnetic or neural system

$$H = -1/2 \sum J_{ij} S_i S_j ,$$

reflecting, in essence, the Ising Model [9].

In this model, the dynamics of the variable S_i are given by the local field

$$B_i = \sum J_{ij} S_j .$$

In the Ising model this field is magnetic; in neural networking, this field represents the electric potential of neural cells.

The "spin flip" or "firing" is determined by

$$S_i = \text{sign}(B_i) ;$$

thus

$$H = -1/2 \sum B_i \text{sign}(B_i) .$$

For the frustration model, F can be written as

$$F = \sum (D_{ij} - I_{ij})^2 = \sum D_{ij} (D_{ij} - 2I_{ij}) + \sum I_{ij}^2 .$$

$\sum I_{ij}^2$ is just a constant, used for normalization and possibly defining temperature. Calling $d_{ij}=(I_{ij} - D_{ij})$, D_{ij} becomes $I_{ij} - d_{ij}$. It is easy to prove that

$$F = - \sum (I_{ij} + d_{ij}) (I_{ij} - d_{ij}) + \text{const} = - \sum d_{ij}^+ d_{ij}^- + \text{const} ,$$

where $d_{ij}^\pm = I_{ij} \pm d_{ij}$. This expression is similar to the Hamiltonian for the Ising model. Note that $d_{ij}^\pm$ is a discrete variable, since the distance between neighboring cells is discrete in this frustration model.

CHAPTER 3

RESULTS

INITIAL RESULTS

Systematic studies of various versions of the frustration model have been performed for this research. The versions studied using Algorithm 1 include:

- models with or without "frozen" (non-movable) characters,
- versions where the characters are allowed to stop once they find their minimum frustration, and
- versions that require the characters to continue moving.

Two models, one with finite and one with infinite boundaries, included temperature (Algorithm 2).

All versions were tested using different values of N and different ideal distance matrices with elements I_{ij} ($i=1$ to N , $j=1$ to N).

All these versions are "capitalistic" versions; each character minimizes its own frustration without considering the frustration of the system as a whole. A "socialistic" version is being developed, where all the characters must minimize the whole system's frustration. In each case, the mean and total frustration, and the standard deviation, were calculated.

The versions with no boundaries deserve a special remark. In general, most computational simulation studies are performed with periodic boundary conditions. These requirements have the advantage of eliminating edge effects, which are encountered in the finite non-periodic boundary versions, and can completely dominate very small systems (surface effects). The disadvantages of the periodic boundaries are that they tend to favor clustering when that may not be the case. This problem, however, is not encountered in the no-boundaries case. In the infinite boundaries case, the characters may drift off, or travel in a straight line clustered together with a constant velocity, as will be discussed below.

In versions where frozen characters are present, the moving characters move around the frozen ones in different patterns. In versions where no frozen characters are present, the characters move in clusters (or "shape changing" clusters) through space, especially when no boundaries exist. When non-periodic boundaries are present, the characters bounce off the walls.

The matrix I_{ij} can reflect patterns that model different behaviors in natural systems. This matrix represents the amount of disorder and frustration imposed upon the system. Preferred separations can be:

- all alike ($I_{ij} = \text{constant for all } i \neq j$);
- random (I_{ij} 's are chosen randomly for $i \neq j$);
- approach-avoidance ("A" prefers a small separation from "B", but "B" prefers a large separation from "A");

-- groupings of like characteristics.

When $T=0$, observations indicate four possible states of the system, which we call "stability," "relative stability," "relative instability," and "instability." Since a character is allowed to stop if moving would increase its frustration, the entire system can come to a state of minimum frustration and freeze into a stationary, stable final state. In the relatively stable final state, some characters move back and forth, oscillating about a minimum total frustration. This is called a "shuttle."

When a system has relaxed to relative instability, character locations and their total frustration cycle over a large number of iterations near the minimum value of total frustration. Since characters move in accordance with minimizing their own frustration, the total frustration of the system can increase because the optimum move can increase the frustration of many characters' neighbors.

For random I_{ij} 's, the frustration is such that the system never settles down, even for $T = 0$. However, the frustration oscillates around one value with a superposition of a few frequencies.

In order to explore the possibilities of the model, several different cases with no particular relationship to each other were studied. Unfortunately, the number of possibilities that can be studied with both algorithms is immense. Therefore, the possibilities must be narrowed.

ZERO TEMPERATURE RESULTS

With Algorithm 1 ($T=0$), the relaxation in time towards "equilibrium" was in most cases nearly exponential.

$$\underline{I_{ij} = 5}$$

Fig. 1. The logarithm of total frustration for selected number of characters versus the number of iterations or time steps is shown. The ideal distance matrix values for the character in each system was always the same and equal to 5. For details see text.

This can clearly be seen in Figure 1, where the logarithm of total frustration for selected number of characters versus time is depicted [15]. For all these cases there is one "frozen" character present. The ideal distance elements were all taken to be equal to 5.

This figure also shows that the total frustration increases with the number of characters. The relationship between the total frustration and the number of characters appears to be

$$\text{Total Frustration} \cong \text{const} * N^{2+x}$$

where x is a number between 0 and 1, most likely close to 0.4.

In Fig. 2, one can see three time intervals with different behavior of the frustration of one character [16,17].

For this case, a group of five movable characters and one frozen character ($N=5$, $M=1$), for which the ideal distance matrix elements I_{ij} were taken at random such that $|I_{ij}| < 15$, the frustration behavior of each character (individual character's frustration) has been investigated in detail. In the first few iterations, nearly exponential relaxation is found as discussed above; during an intermediate time period quasi-periodic behavior can be seen. After 100 iterations, a periodic pattern emerges and is observed. At these times, the characters are running around the frozen character in a circular fashion.

$$\underline{N=5} \quad \underline{M=1} \quad \underline{\text{RANDOM } I_{ij} < 15}$$

Fig. 2. The logarithm of the frustration of an individual character versus time in a party of five characters and one frozen character is shown. The matrix elements I_{ij} are random and smaller than 15. Clearly, three different time dependences can be seen in time space; for more detail, see text.

An interesting physics by-product was obtained in testing the program using regular polygons such as triangles, squares, parallelograms, and hexagons, for which I_{ij} can be calculated [18]. In all cases studied and tested, the characters stopped or

performed a "shuttle" motion with two, three, or more repeating patterns, respectively.

When no frozen characters are present, and all ideal distances are equal, the characters form regular geometric patterns, similar to the case mentioned above. A triangle is formed when $N = 3$, a parallelogram when $N = 4$, and so on. As N increases, patterns within patterns are formed. When $N=7$, for example, a hexagon with the seventh character in the center was observed. With further increasing N , cluster formations appear.

The result of regular patterns suggested the idea that this model could generate similar results to those published by F.S. Lestingi [19] on the experimentally created "Thompson" patterns. The triangle, square, and pentagon are atomic "plum pudding" solutions with 3, 4, and 5 electrons in a uniform sea of positive charge. These equilibrium arrangements were obtained by floating magnets in a dish of water. A similar experiment on a larger scale is being developed at the Exploratorium [20]. Computationally, for $N > 5$, more than one "equilibrium" solution, which is sometimes not the same as that experimentally obtained, have been found.

In Figs. 3a and b [17], and Fig. 4 [21], patterns depicted are obtained after about sixty iterations (time steps) for all I_{ij} elements equal to 10, 50 and 1, respectively; the number of characters is 100 (400). These pictures show condensed-matter like features such as clustering effects and glassy-like pattern formation. The circles in Figure 3b occur spontaneously; these

normally occur with a permanent frozen character in the center. These same results have been found by different methods in a two dimensional continuum space where the interactions between particles obey a Hooke's law [22].

At first, the appearance of the right-angled arms of the regular shape in Fig. 4, was thought to be due to lattice effects, since the limiting case $I_{ij}=1$ had been considered. However, after applying simulated annealing, the system relaxed to a configuration with a much lower minimum, shaped in a circular cluster like in the case of Figs. 3. This is a clear indication of the multivalley structure of the frustration space, since the armed shaped configuration was just stuck in a local minimum of frustration with high barriers. The system did not have enough energy to "jump off" the minimum. Once simulated annealing was applied, that is when heating and subsequent cooling of the system was introduced, the system was allowed to overcome the frustration barrier and the arms actually "melted down."

N=100 Iij=10 IT=56

MEAN FRUSTRATION=0.15723E+04

Fig. 3a. The initial positions (x's) and the obtained pattern (dots) after about 60 iterations (time steps) of a party of 100 characters with $|I_{ij}|=10$ are depicted. Clustering effects are observed. For more detail see text.

N=100 I_{ij}=50 IT=56

MEAN FRUSTRATION=0.12387E+04

Fig. 36. The initial positions (x's) and the obtained pattern (dots) after about 60 iterations (time steps) of a party of 100 characters with $|I_{ij}|=50$ are depicted. Amorphous-like lattice formation is observed. For more detail see text.

Fig. 4. The initial positions (x's) and the obtained pattern (dots) after 61 iterations (time steps) of a party of 400 characters with $|I_{ij}|=1$ are depicted. For details see text.

Using infinite boundaries becomes important in the case of approach-avoidance, when $I_{ij} = C1$ but $I_{ji} = C2$, where $C1$ is small but $C2$ is large. If there are no boundaries, the system moves linearly in a cluster with constant velocity. This can be seen in Fig. 5, where the patterns obtained after 91 and 100 iterations show the way the system of 20 particles clustered in a single configuration moves in a straight line.

This is an indication of the fact that just as for neural systems, the dynamical properties of a system are much richer than the dynamical properties of systems with symmetric pairwise interactions. This was also the case in Fig. 2. The asymmetric cases, therefore, should be studied in more detail using the general framework of nonlinear dynamics.

$N=20$ $I_{ij}=1$ $I_{ji}=50$
 $IT=100$ MEAN FRUSTRATION=17076.36

Fig. 5. The initial positions (x's) and the obtained patterns after 91 (filled dots) and 100 (empty dots) iterations (time steps) of a party of 20 characters with asymmetric pairwise interactions ($|I_{ij}|=1$, $|I_{ji}|=50$) are depicted. For details see text.

When Algorithm 2 was used, for $T=0$, the initial relaxation was again nearly exponential, although this is debatable, as Figs. 6a and 6b show.

Fig. 6a. The initial relaxation of the logarithm of total frustration for 100 characters versus the number of iterations or time steps is shown. The ideal distance matrix values were the same for all characters and equal to 5. For details see text.

Fig. 6b. The initial relaxation of the logarithm of total frustration for 100 characters versus the number of iterations or time steps is shown. The ideal distance matrix values were the same for all characters and equal to 5. For details see text.

These figures show the initial relaxation of total frustration of a party of 100 mobile characters, with no frozen characters, for which the ideal distances were equal to 5, with respect to time. The same behavior is observed for any number of characters N without changing any other parameters. Once the system relaxed,

the plot shows that the total frustration remains constant. This can be seen in Fig. 7, where the logarithm of total frustration versus iterations or time steps is shown for $N=5, 10, 20, 50, 100$, and 200. Again $I_{ij}=5$ for all cases and $T=0$.

Fig. 7. The logarithm of total frustration for selected number of characters versus the number of iterations or time steps is shown. The ideal distance matrix values for the character in each system was always the same and equal to 5. For details see text.

The initial relaxation is nearly exponential, although not as clear as for the case of Fig. 1. Two different exponential behaviors can almost be seen, although again this is debatable, one exponential which goes until about 100 iterations, and another after that until the frustration reaches the "equilibrium" value.

The difference between the cases in Fig. 1 and Fig. 7 is not completely clear yet. Likely, the discrepancy is due to the difference in algorithm. The behavior depicted in Fig. 1 deals with Algorithm 1, which probably makes this frustration behavior smoother since the system goes directly, at $T=0$, to its minimum frustration in a steepest descent way. Figure 7 was obtained with Algorithm 2 which might be rejecting a lot of moves, since a character selects a neighbor at random to move, so the algorithm does not go as fast.

Figure 8 shows the dependence of the total frustration with the number of characters in cases where all the ideal distance matrix elements were equal to 5 and $T=0$. A power law fit was performed and the result predicts that the total frustration is proportional to the number of characters to the power 2.426, in accordance with Fig. 1.

Fig.8. The total 'equilibrium' frustration versus the number of characters is shown. The interaction between characters (ideal distance matrix elements) for each system (each dot in the figure) was the same for all characters and equal to 5. A power fit was performed, where y represents frustration and x represents the number of characters, giving a power of 2.426. For more details see text.

TEMPERATURE EFFECTS.

A major interest in this research was to study the temperature effects of the frustration model and whether or not a phase transition could be generated. If a critical point existed, it would be interesting to see indications of precursor effects and if the transition would be of first or second order.

Temperature was incorporated in Algorithm 1 by means of the Metropolis algorithm as explained in Chapter 1, giving Algorithm 2. As expected, with increasing temperature, more thermal motion is introduced. In analogy with the Ising model, temperature may be defined in units of $\sqrt{\langle I_{ij}^2 \rangle}$. Presently, temperature is expressed in individual frustration units.

Temperature studies showed the following unusual observations. In the case of regular polygons, a shuttle stays a shuttle, when one character is permanently frozen. For random I_{ij} 's, at $T=0$, there are discrete layers of frustration, separated by more than one standard deviation in frustration. This effect disappears at "hot" temperatures, where the running average of all characters are about the same. Further work, with a focus on T-dependent clustering effects, is in progress.

Using Algorithm 2 (Appendix C), clear indications of a critical point were observed.

Figure 9a shows a plot of Δ (explained in Chapter 1) versus temperature for when the system is heated from $T=0$ to $T=5$, where the changes in temperature are in steps of $\Delta T=0.05$. The system in this case consists of 50 mobile particles, with ideal distance elements equal to 5.

A clear transition can be seen for $T \approx 2$, temperature for which the behavior of Δ changes drastically from zero to higher values. The part of the curve above $T=2$ might get smoothed out if the average was taken over a larger number of points (≈ 250 was the number of points taken).

Fig.9a. The standard deviation of the average total frustration versus temperature is depicted, for a system of 50 characters, in a heating process with a temperature interval of 0.05. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Fig.9b. The standard deviation of the average total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.05. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Figure 9b shows the plot for Δ with the same parameters as Fig. 9a, but in this case the system is cooled from $T=5$ to $T=0$, with an interval change in temperature of $\Delta T=-0.05$. Again the transition occurs at $T \approx 2$.

Figure 10a shows the plot of the average frustration $\langle F \rangle$ (defined above) versus temperature in the heating process with $\Delta T=0.05$.

Fig.10a. The average total frustration versus temperature is depicted, for a system of 50 characters, in a heating process with a temperature interval of 0.05. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Once more a phase transition can be seen at $T \approx 2$. The jump at $T \approx 1$ cannot be considered a critical point since this behavior only demonstrates the multivalley qualities of the frustration state space, as one can determine looking at Fig. 10b for the cooling process ($\Delta T = -0.05$), where such a jump does not exist.

Fig.10b. The average total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.05. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

The jump observed in the heating process (Fig. 10a) can be explained by noticing that since the system started at low temperatures, and slowly moved up in temperature, the system could have easily gotten "stuck" in a higher local minimum.

When the temperature is raised, the system has more energy to look for lower minima, and in fact this is what happened after $T \approx 1$. The system obtained enough energy to jump off the local minimum and find a lower one.

Similar situations are encountered in the plots of the minimum frustration $F_{\min}$ versus temperature, in the heating ($\Delta T = 0.05$) and cooling ($\Delta T = -0.05$) processes, which can be seen in Figs. 11a and 11b, respectively.

After the transition, Figs. 11a and 11b show that the values of $F_{\min}$ do not always go up with temperature. This is due to the fact that for each temperature, that is after 600 iterations were taken to relax the system in these plots, a different value of $F_{\min}$ is computed. What happens then is that for high temperatures ($T > 2$) the system has more thermal energy to explore different configurations. The system can actually find a configuration with a low frustration, but due to its high energy, the system will not stay in one particular minimum. The system wanders around between different minima without settling in any of them.

Fig.11a. The minimum total frustration versus temperature is depicted, for a system of 50 characters, in a heating process with a temperature interval of 0.05. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Fig.11b. The minimum total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.05. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

The interval in temperature chosen seems to be of great importance. The faster the system is heated or cooled, the larger the temperature at which the phase transition occurs. This can be seen in Figs. 12, 13a and 13b, for which the transition occurs at $T \approx 2.6$.

Fig.12. The standard deviation of the average value of total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.1. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Another curious difference can be seen in Fig. 13a with respect to Fig. 10a. Figure 13a shows two jumps before the critical temperature. An explanation could be that the faster the heating, the more energy the system acquires, and therefore an earlier jump to a lower minimum occurs, although still not the lowest.

Fig.13a. The average value of total frustration versus temperature is depicted, for a system of 50 characters, in a heating process with a temperature interval of 0.1. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Fig.136. The average value of total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.1. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

The number of characters is another important factor in the determination of the phase transition. The critical temperature increases with the number of characters.

An example of this can be seen in Figs. 14a and 14b for systems of 100 characters.

Fig.14a. The standard deviation of the average value of total frustration versus temperature is depicted, for a system of 100 characters, in a heating process with a temperature interval of 0.5. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

Fig.14b. The average value of total frustration versus temperature is depicted, for a system of 100 characters, in a heating process with a temperature interval of 0.5. The interaction between characters (ideal distance matrix elements) is the same for all characters and equal to 5. For details see text.

As Figs. 14a and 14b show, there is no definite feature that tells whether or not the transition has been completed. Extending the computation over higher temperatures is necessary. This is especially clear in Fig. 14b, since the system jumps two times to "better" minima in the same way that the 50 character systems of

Figs. 10a and 13a did. However, the almost chaotic behavior that followed such jumps in those two figures is not shown in Fig. 14b. Fig. 14a shows an unusual sharp jump at $T=5$, which is precisely the same temperature at which the first jump in Fig. 14b occurs. A more subtle change in behavior occurs at $T \approx 10$ which coincides with the second jump in Fig. 14b.

Fig.15. The the standard deviation of the average value of total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.05. The interaction between characters (ideal distance matrix elements) is taken at random to be less than 15. For details see text.

Qualitatively different behaviors are observed when the ideal distance matrix elements are not all the same. This is shown in Figs. 15 and 16, where the number of characters is 50 and the ideal distance elements are taken at random and taken to be less than 15.

Fig.16. The average value of total frustration versus temperature is depicted, for a system of 50 characters, in a cooling process with a temperature interval of -0.05. The interaction between characters (ideal distance matrix elements) is taken at random to be less than 15. For details see text.

These two figures show the cooling behavior when the temperature interval is $\Delta T = -0.05$. In Fig. 15, the transition temperature seems to be at $T \approx 0.6$, although the values of Δ for higher temperatures keep falling down to zero, which may indicate that in reality the transition does occur at a higher value of T . The behavior is much different in Fig. 16 compared with the cases studied earlier for $I_{ij} = 5$. Figure 16 shows the dependence of $\langle F \rangle$ with temperature with the same parameters as in Fig. 15. There seems to be no defined transition in this case. However, the low valley occurring at $T \approx 1$ is quite surprising and more work is needed to obtain a convincing explanation.

CHAPTER 4

APPLICATIONS

SPIN-CLUSTER EFFECTS IN SPIN GLASSES

Experimental as well as theoretical reviews [7,23] of spin-glass investigations suggest that, despite the progress made, the physical origin of spin-glass freezing is not yet completely understood. Mean-field theory does not appear to generate satisfactory interpretations for the freezing process [23,24]. Clustering and frustration are difficult to describe using a mean-field approach. The main reason is that a mean value in a random (spin) system is not always the most probable one. It may be more useful to describe and understand random disordered frustrated systems by using a method involving most probable values for critical and physical parameters. A different theoretical approach is needed to investigate the non-linear physics aspects found in experimental glass systems.

Some single-crystal studies in Oxide-Spin-Glass systems such as $\text{Fe}_{2-x}\text{Ti}_{1+x}\text{O}_5$ [25] may help address some of these problems. Members of the uniaxial oxide-spin-glass system $\text{Fe}_{2-x}\text{Ti}_{1+x}\text{O}_5$ (pseudobrookite) are insulating or semiconducting oxides, showing unusual anisotropic spin-glass properties well below room temperature (RT) [26]. At T_g , which is about 55K for $x = 0$, the c-axis magnetic susceptibility exhibits a cusp, while the

perpendicular components show paramagnetic behavior until about 10 K. Single-crystal muon-spin-relaxation (μ SR) experiments clearly indicate the appearance of spin clusters just above T_g [27,28]. The muon is expected to behave as in well-known magnetic oxides, where μ -O bonding occurs [29,30]. In essence, the positive muon probes the internal magnetic field at its stop site. The observed cluster effects can be interpreted [31] in terms of a Griffiths-like phase occurring in a small temperature region just above T_g where non-exponential spin relaxation occurs. The occurrence of a Griffiths temperature region reflects precursor effects signaling the onset of a spin-glass phase transition. Recent transverse (TF) and zero-field (ZF) μ SR and Moessbauer Effect Spectroscopy (MES) on single crystals of $\text{Fe}_{2-x}\text{Ti}_{1+x}\text{O}_5$ ($x = .25$) [25] also show the occurrence of spin clusters in the freezing process. Frustration is an important ingredient in the interpretation of such results.

FRUSTRATION IN SPIN GLASSES

As discussed earlier in this thesis, frustration gives rise to a multidegenerate ground state. The configuration space is conformed of many valleys separated by energy barriers. Each one of these valleys represents a possible macrostate or "frozen" state of the system. However, these states will only be temporary unless the barriers are effectively infinite. If the barriers are

finite, eventually the spin system will "jump" from valley to valley if a long enough time scale is considered. For low enough temperatures, these dynamical spin processes occur on a time scale so big compared to observation times that the probability that the system would "flip" to a nearby valley becomes insignificant. For sufficiently high temperatures, this probability becomes significant enough to produce noticeable changes in the spin system. Above a certain critical temperature, the system jumps from valley to valley in a time scale comparable to observation times. This is similar to what has been shown in Chapter 2 in the temperature results of the frustration model.

The transition region of any disordered spin system displaying broken ergodicity has not yet been satisfactorily understood. The results obtained so far with the frustration model indicate this is probably the correct procedure for developing an understanding of the problem.

The frustration model presented in this thesis is similar to but more general than the Ising model [17]. As has been shown in Chapter 2, the relaxation in time towards thermal "equilibrium" is at early times nearly exponential. In the case where the matrix element I_{ij} is random, at zero temperature, after a sufficiently long time, a periodic motion pattern emerges; during an intermediate time period, quasiperiodic behavior is observed. At sufficiently high temperatures, only quasiperiodic behavior is seen after the initial exponential relaxation. At even higher temperatures, only exponential behavior is seen at early times,

after which only random motion occurs. This frustrated process may be similar to the freezing process in spin glasses. The quasi periodicity observed with the frustration model, as well as the experimental observance of spin clustering just above T_g , can be seen as precursor effects signaling the onset of the spin-glass phase transition.

Further work is in progress, such as applying the model with I_{ij} representing competing dipolar interactions in the insulating spin-glasses like pseudobrookite, or representing RKKY interactions for the metallic spin-glasses. Based upon earlier frustration results obtained with this model, a reasonable interpretation of the spin-freezing process as a good possibility to improve the understanding is anticipated.

In conclusion, magnetic resonance measurements have indicated the occurrence of spin clustering in the anisotropic spin glass pseudobrookite just above the spin-glass temperature. An interpretation can be found in recently developed theoretical approaches in terms of spin clustering [24,32,33]. Along similar lines, spin-cluster formation can be understood in terms of the frustration model presented here and in reference [17].

Non-exponential relaxation in spin-glasses and structural glasses occurring just above T_g has been addressed by Campbell et al. [34] in terms of configuration space morphology. As microscopic features in these glasses differ basically, the common qualitative characteristics such as "clustering" and "frustration" indicate more than resemblance at fundamental level.

HIGH-T_c VORTEX BEHAVIOR

Muon Spin Relaxation results may indicate that magnetic frustration can be a key concept in addressing the physical origin of the superconductivity of novel high-T_c oxide cuprates of the type $\text{RBa}_2\text{Cu}_3\text{O}_7$, where R is the symbol for a rare earth except Pr [35]. Frustration patterns obtained with the frustration model presented here may resemble the fluid-like properties of the vortex state of such oxide superconductors. To what extent this is true and what types of patterns should be used is still unclear. Further study is under way [36].

CHAPTER 5

CONCLUSION

In an attempt to describe frustration in natural disordered systems, the Gold model [11] was taken as a starting point and essential modifications were made to describe the physical concepts used in frustration.

One of the fundamental problems in the theory of condensed matter is to understand the macroscopic properties of a system in terms of the interparticle interactions. Along similar lines, central to the frustration model is the ideal separation matrix I_{ij} . This matrix determines whether, after initial exponential relaxation, periodic oscillations and motion or apparently random motion occur, or if patterns form among characters. Regular polygons and structures like Thompson's "plum pudding" atomic patterns can be generated with specific regular I_{ij} 's. Clustering effects have been observed at "low" temperatures for random I_{ij} 's and regular small I_{ij} 's. Indications of precursor effects signaling the onset of the "freezing process" showed up in individual frustration behavior. Frustration is an important concept in glass and spin-glass science.

The frustration model is similar to but more general than the well-known Ising model, which has been used in spin-glass, glass and neural network studies. The major difference is that the Ising model operators S_i have two values ± 1 ; in the frustration model,

the discrete parameter $d_{ij}^{\pm}$ has an infinite number of discrete values.

The results obtained so far indicate that this approach may be the right direction towards describing frustration origins for natural disordered systems.

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APPENDIX A

The question of whether one should take F to be:

$$F = \sum_{ij} (D_{ij} - I_{ij})^2 \quad \text{or} \quad F_{tjh} = 1/2 \sum_{ij} [(D_{ij} - I_{ij})^2 + (D_{ij} - I_{ji})^2]$$

to take into account cases where $I_{ij} \neq I_{ji}$ has been raised [18]. Note that $D_{ij} = D_{ji}$.

However, these expressions are exactly the same, as can be shown:

$$\begin{aligned} F_{tjh} &= 1/2 \sum_i \sum_j [(D_{ij} - I_{ij})^2 + (D_{ij} - I_{ji})^2] = \\ &= 1/2 \left[\sum_i \sum_j (D_{ij} - I_{ij})^2 + \sum_i \sum_j (D_{ji} - I_{ji})^2 \right] = \\ &= 1/2 \left[\sum_i \sum_j (D_{ij} - I_{ij})^2 + \sum_j \sum_i (D_{ij} - I_{ij})^2 \right] = \\ &= 1/2 \left[\sum_i \sum_j (D_{ij} - I_{ij})^2 + \sum_i \sum_j (D_{ij} - I_{ij})^2 \right] = \\ &= \sum_i \sum_j (D_{ij} - I_{ij})^2 = F \end{aligned}$$

where the facts that $D_{ij} = D_{ji}$ and that $\sum_i$ and $\sum_j$ commute have been taken into account.

APPENDIX B

Note that the program presented in this Appendix and the one presented in Appendix C contain a great deal of related calculations which make them extremely sensible to round-off error. Therefore it is very important to use double precision to make the final solution a bit more accurate.

PROGRAM MSFRUST

```
C THIS PROGRAM MOVES THE CHARACTERS (N) ACCORDING TO
C MINIMIZING A CHARACTER'S INDIVIDUAL FRUSTRATION:
C  $F_i = \text{SUM}(D_{ij} - I_{ij})^2$ 
C WHERE THE SUM IS OVER j. IT PICKS ONE OF THE EIGHT SPACES
C IN A MOORE NEIGHBORHOOD AT RANDOM, AND PERFORMS A
C MONTE CARLO SIMULATION, WITH A BOLTZMAN PROBABILITY
C DISTRIBUTION.
C THERE ARE NO BOUNDARIES.
C THERE ARE NO FROZEN CHARACTERS. THIS CAN EASILY BE
C CHANGED.
C ID(I,J) IS TAKEN TO BE EQUAL FOR ALL I,J. THIS CAN EASILY BE
C GENERALIZED TO DIFFERENT VALUES.
C THE PARAMETERS ARE SET AT THE BEGINNING OF THE PROGRAM
C AND CAN BE EASILY ALTERED TO MEET ANY SPECIFICATION.
C IT PRINTS OUT THE FRUSTRATION OF TWO INDIVIDUAL
C CHARACTERS FOR EACH ITERATION, AS WELL AS THE TOTAL
C FRUSTRATION.
C FOR EACH ITERATION, IT KEEPS TRACK OF THE MINIMUM VALUE
C OF TOTAL FRUSTRATION OBTAINED IN THE PRECEDING
C ITERATIONS.
C IF N IS CHANGED, REMEMBER TO CHANGE FORMATS 23 AND 80
C ACCORDINGLY!

PARAMETER(NMAX=110)
INTEGER X(NMAX),Y(NMAX),XNEW,YNEW,IQUEEN(8,2)
DIMENSION FOLD(NMAX),RN(NMAX),ID(NMAX,NMAX)
DOUBLE PRECISION TFOLD,FOLD,TOTFMIN,DNEW,FNEW,TOTF
```

DATA IQUEEN/1,1,1,0,0,-1,-1,-1, 1,0,-1,1,-1,1,0,-1/

C INITIAL PARAMETERS USED TO START CALCULATIONS (THEY
C CAN BE VARIED ACCORDINGLY TO CASE STUDIED):
C N IS THE NUMBER OF CHARACTERS.
C M IS THE NUMBER OF TOTAL ITERATIONS DESIRED.
C D IS THE CONSTANT WHICH DETERMINES THE IDEAL DISTANCE
C BETWEEN CHARACTERS.
C T IS THE TEMPERATURE AT WHICH THE RELAXATION TO THE
C MINIMUM FRUSTRATION IS DESIRED.
C IMAX AND JMAX DETERMINE THE INITIAL RECTANGLE (SQUARE)
C WHERE THE INITIAL POSITIONS OF THE CHARACTERS ARE TO
C BE RESTRICTED TO.
C ISEED IS A CONSTANT USED TO START UP THE RANDOM
C GENERATOR [13]

ISEED=9352
N=100
M=600
D=5
WRITE(*,*) "INPUT TEMPERATURE T"
READ(*,*) T
IMAX=100
JMAX=100
ISEED=-IABS(ISEED)

C OPEN A FILE THAT WILL CONTAIN THE INITIAL POSITIONS OF THE N
C CHARACTERS

OPEN(UNIT=11,FILE='FRUSXY.IN')

C LOOP TO INITIALIZE THE IDEAL DISTANCE MATRIX. IN THIS CASE THEY
C ARE EQUAL TO A CONSTANT D. THIS CAN BE EASILY GENERALIZED TO
C ANY OTHER CASE.

DO 15 I=1,N
DO 10 J=1,N
IF(I.EQ.J) THEN
ID(I,J)=0
GO TO 10
ENDIF
ID(I,J)=D

```

10    CONTINUE
15    CONTINUE

C  LOOP TO INITIALIZE THE POSITIONS OF THE CHARACTERS AND WRITE
C  THEM INTO THE FRUSXY.IN FILE FOR POSTERIOR USE.

      DO 20 I=1,N
        X(I)=1+RAN(ISEED)*IMAX
        Y(I)=1+RAN(ISEED)*JMAX
        WRITE(11,*) X(I),Y(I)
20    CONTINUE

      CLOSE(11)

C  INITIALIZE EACH INDIVIDUAL CHARACTER'S FRUSTRATION FOLD(I)
C  AS WELL AS THE TOTAL FRUSTRATION TFOLD.  INITIALIZE THE TOTAL
C  MINIMUM FRUSTRATION FOR FURTHER COMPARISON.

      TFOLD=0
      DO 30 I=1,N
        FOLD(I)=0
        DO 25 J=1,N
          IF(I.EQ.J) GO TO 10
          DIJ=SQRT(FLOAT((X(I)-X(J))**2 + (Y(I)-Y(J))**2))
          FOLD(I)=FOLD(I)+(DIJ-ID(I,J))**2
25    CONTINUE
        TFOLD=TFOLD+FOLD(I)
30    CONTINUE
      TOTFMIN=TFOLD

C  OPEN DATA FILES WHICH WILL CONTAIN THE VALUES OF INDIVIDUAL
C  CHARACTER'S FRUSTRATION, TOTAL FRUSTRATION, AND MINIMUM
C  FRUSTRATION FOR EACH ITERATION AS WELL AS THE LAST POSITIONS
C  OF THE CHARACTERS UPON RELAXATION.

      OPEN(UNIT=12,FILE='FRUS.OUT')
      OPEN(UNIT=14,FILE='FRUSXY.OUT')

C  MAJOR LOOP OVER DESIRED NUMBER OF ITERATIONS UNTIL RELAXATION
C  TO FINAL CONFIGURATION.

      DO 100 IT=1,M

```

C LOOP TO CHOOSE ONE CHARACTER AT RANDOM AND MOVE IT IF ALGORITHM
C INDICATES TO DO SO.

DO 55 K=1,N

C CHOOSE A CHARACTER AT RANDOM. IF ALREADY CHOSEN, CHOSE
C ANOTHER.

```
3 5      RN(K)=N*RAN(ISEED)+1
        DO 40 L=1,K-1
            IF(RN(K).EQ.RN(L)) GO TO 35
4 0      CONTINUE
```

C CHOOSE ONE OF THE 8 NEIGHBORING SPACES AT RANDOM.

```
        IJUNK=8*RAN(ISEED)+1
        ISTP=IQUEEN(IJUNK,1)
        JSTP=IQUEEN(IJUNK,2)
        XNEW=X(RN(K))+ISTP
        YNEW=Y(RN(K))+JSTP
```

C IF THAT POSITION IS ALREADY TAKEN SKIP CALCULATION FOR
C PRESENT CHARACTER AND CHOOSE ANOTHER CHARACTER (START
C K LOOP AGAIN).

```
        DO 45 L=1,N
            IJUNK=IABS(X(L)-XNEW)+IABS(Y(L)-YNEW)
            IF(IJUNK.EQ.0) GO TO 55
4 5      CONTINUE
        FNEW=0
```

C CALCULATE THE INDIVIDUAL CHARACTER'S FRUSTRATION IN
C POTENTIAL NEW POSITION.

```
        DO 50 J=1,N
            IF(J.EQ.RN(K)) GO TO 50
            DNEW=SQRT(FLOAT((XNEW-X(J))**2+(YNEW-Y(J))**2))
            FNEW=FNEW+(DNEW-ID(RN(K),J))**2
5 0      CONTINUE
```

C CALCULATE THE DIFFERENCE BETWEEN THE NEW AND THE OLD

```

C  INDIVIDUAL FRUSTRATIONS DELTAF.
C    IF DELTAF<0 MOVE CHARACTER
C    IF DELTAF>0 THEN
C      CALCULATE P=EXP(-DELTAF/T)
C      IF P<TOL (RANDOM VARIABLE BETWEEN 0 AND 1) STAY
C      IF P>TOL MOVE.
C  NOTE: IF T=0 THEN IF DELTAF>0 STAY.

```

```

      DELTAF=FNEW-FOLD(RN(K))
      IF(DELTAF.LT.0) THEN
        FOLD(RN(K))=FNEW
        X(RN(K))=XNEW
        Y(RN(K))=YNEW
      ELSE
        IF(T.EQ.0) THEN
          P=0
        ELSE
          P=EXP(-DELTAF/T)
        ENDIF
        TOL=RAN(ISEED)
        IF(P.GT.TOL) THEN
          FOLD(RN(K))=FNEW
          X(RN(K))=XNEW
          Y(RN(K))=YNEW
        ENDIF
      ENDIF

```

```

55    CONTINUE

```

```

C  COMPUTE THE NEW TOTAL FRUSTRATION.

```

```

      TOTF=0
      DO 65 I=1,N
        DO 60 J=1,N
          IF(I.EQ.J) GO TO 60
          DIJ=SQRT(FLOAT((X(I)-X(J))**2+(Y(I)-Y(J))**2))
          TOTF=TOTF+(DIJ-ID(I,J))**2
60      CONTINUE
65    CONTINUE
      IF(TOTF.LT.TOTFMIN) TOTFMIN=TOTF

```

TFOLD=TOTF

C WRITE RESULTS TO DATA FILE.

```
      WRITE(12,70) IT,FOLD(2),FOLD(4),TFOLD,TOTFMIN
70    FORMAT(' ',I4,2F12.2,2F16.2)
```

100 CONTINUE

C AFTER MAJOR LOOP IS OVER (AFTER M ITERATIONS) WRITE

C FINAL CONFIGURATION (CHARACTER'S POSITIONS) TO DATA FILE.

```
      DO 80 I=1,N
        WRITE(14,*) X(I),Y(I)
80    CONTINUE
```

```
      CLOSE(12)
      CLOSE(14)
90    CONTINUE
```

END

C RANDOM GENERATOR [13].

FUNCTION RAN(IDUM)

```
PARAMETER(M=714025,IA=1366,IC=150889,RM=1.4005112E-6)
SAVE IR,IY
DIMENSION IR(97)
```

```
IF(IDUM.LT.0) THEN
  IDUM=MOD(IC-IDUM,M)
  DO 11 J=1,97
    IDUM=MOD(IA*IDUM+IC,M)
    IR(J)=IDUM
11  CONTINUE
    IDUM=MOD(IA*IDUM+IC,M)
    IY=IDUM
ENDIF
J=1+(97*IY)/M
IF(J.GT.97.OR.J.LT.1)PAUSE
```



```
IY=IR(J)
RAN=IY*RM
IDUM=MOD(IA*IDUM+IC,M)
IR(J)=IDUM
```

```
RETURN
```

```
END
```

```
*****
```

APPENDIX C

PROGRAM MSFRUST2

PARAMETER(NMAX=400)
INTEGER X(NMAX),Y(NMAX),XNEW,YNEW,IQUEEN(8,2)
DOUBLE PRECISIONFAVER,FSQAVAR,TFOLD,TOTF
DOUBLE PRECISION TOTFMIN,FOLD,FNEW,DELTA
DIMENSION FOLD(NMAX),RN(NMAX),ID(NMAX,NMAX)
DATA IQUEEN/1,1,1,0,0,-1,-1,-1, 1,0,-1,1,-1,1,0,-1/

ISEED=3587
ITAVAR=350
N=100
M=600
D=5
IMAX=100
JMAX=100
ISEED=-IABS(ISEED)

OPEN(UNIT=11,FILE='FRUS4XY.IN')

DO 3 I=1,N
DO 2 J=1,N
ID(I,J)=D
2 CONTINUE
3 CONTINUE

DO 5 I=1,N
6 X(I)=1+RAN(ISEED)*IMAX
Y(I)=1+RAN(ISEED)*JMAX
DO 4 J=1,I-1
IF(X(I).EQ.X(J).AND.Y(I).EQ.Y(J)) GO TO 6
4 CONTINUE
WRITE(11,*) X(I),Y(I)
5 CONTINUE

CLOSE(11)

OPEN(UNIT=12,FILE='FRUS4,20,600,5,.OUT')

```

OPEN(UNIT=14,FILE='FRUS4XY.OUT')

DO 200 T=0.0,15.0,0.5

FAVER=0
FSQAVR=0
TOTF=0
TOTFMIN=0
DELTAf=0

TFOLD=0
DO 20 I=1,N
    FOLD(I)=0
    DO 10 J=1,N
        IF(I.EQ.J) GO TO 10
        DIJ=SQRT(FLOAT((X(I)-X(J))**2 + (Y(I)-Y(J))**2))
        FOLD(I)=FOLD(I)+(DIJ-ID(I,J))**2
1 0    CONTINUE
        TFOLD=TFOLD+FOLD(I)
2 0    CONTINUE
        TOTFMIN=TFOLD

DO 100 IT=1,M

    DO 50 K=1,N

2 5        RN(K)=N*RAN(ISEED)+1
            DO 30 L=1,K-1
                IF(RN(K).EQ.RN(L)) GO TO 25
3 0        CONTINUE

            IJUNK=8*RAN(ISEED)+1
            ISTEP=IQUEEN(IJUNK,1)
            JSTEP=IQUEEN(IJUNK,2)
            XNEW=X(RN(K))+ISTEP
            YNEW=Y(RN(K))+JSTEP

            DO 40 L=1,N
                IJUNK=IABS(X(L)-XNEW)+IABS(Y(L)-YNEW)
                IF(IJUNK.EQ.0) GO TO 50
4 0        CONTINUE
            FNEW=0

```

```

DO 45 J=1,N
  IF(J.EQ.RN(K)) GO TO 45
  DNEW=SQRT(FLOAT((XNEW-X(J))**2+(YNEW-Y(J))**2))
  FNEW=FNEW+(DNEW-ID(RN(K),J))**2
45  CONTINUE

  DELTAF=FNEW-FOLD(RN(K))
  IF(DELTAF.LT.0) THEN
    FOLD(RN(K))=FNEW
    X(RN(K))=XNEW
    Y(RN(K))=YNEW
  ELSE
    IF(T.EQ.0) THEN
      P=0
    ELSE
      P=EXP(-DELTAF/T)
    ENDIF
    TOL=RAN(ISEED)
    IF(P.GT.TOL) THEN
      FOLD(RN(K))=FNEW
      X(RN(K))=XNEW
      Y(RN(K))=YNEW
    ENDIF
  ENDIF

50  CONTINUE

  TOTF=0
  DO 70 I=1,N
    DO 60 J=1,N
      IF(I.EQ.J) GO TO 60
      DIJ=SQRT(FLOAT((X(I)-X(J))**2+(Y(I)-Y(J))**2))
      TOTF=TOTF+(DIJ-ID(I,J))**2
60  CONTINUE
70  CONTINUE
  IF(TOTF.LT.TOTFMIN) TOTFMIN=TOTF
  TFOLD=TOTF

```

C ROUTINE TO CALCULATE AVERAGE FRUSTRATION AND STANDARD
 C DEVIATION.

```

  IF(IT.GT.ITAVER) THEN

```

```

    FAVER=FAVER+TFOLD
    FSQAVR=FSQAVR+TFOLD*TFOLD
ENDIF

```

```

100 CONTINUE

```

```

    FAVR=FAVER/(M-ITAVR)
    FSQAVR=FSQAVR/(M-ITAVR)
    WRITE(12,15) T,FAVER,FSQAVR-FAVER**2,TOTFMIN
15  FORMAT(' ',F4.2,3F16.2)

```

```

200 CONTINUE

```

```

    CLOSE(12)

    DO 120 I=1,N
        WRITE(14,*) X(I),Y(I)
120 CONTINUE

```

```

    CLOSE(14)

```

```

130 CONTINUE

```

```

    END

```

C RANDOM GENERATOR [13].

```

    FUNCTION RAN(IDUM)

    PARAMETER(M=714025,IA=1366,IC=150889,RM=1.4005112E-6)
    SAVE IR,IY
    DIMENSION IR(97)

    IF(IDUM.LT.0) THEN
        IDUM=MOD(IC-IDUM,M)
        DO 11 J=1,97
            IDUM=MOD(IA*IDUM+IC,M)
            IR(J)=IDUM
11  CONTINUE
        IDUM=MOD(IA*IDUM+IC,M)

```

```
      IY=IDUM
ENDIF
J=1+(97*IY)/M
IF(J.GT.97.OR.J.LT.1)PAUSE
IY=IR(J)
RAN=IY*RM
IDUM=MOD(IA*IDUM+IC,M)
IR(J)=IDUM
```

```
RETURN
```

```
END
```

```
*****
```