Capturing the Emergence of Structure in a Two-Dimensional Spin System

Owen Dix

UC Davis, Physics Department

dix@physics.ucdavis.edu

Abstract

This project is an attempt to investigate the structure present in two—dimensional spin systems with various inhomogeneities. While insight was gained into the dependence of $2D$ structure on the geometry of both the system and the tools used to investigate it, these lessons were predominantly learned through failed attempts to characterize the structure. The long run-times involved in the simulations I had written meant that results of the interesting systems were never produced. Yet from comparison to previous successes in the field, I have discovered that these attempts would likely have been qualitative, at best.

Introduction:

For my final project, I have studied the emergence of structure in two—dimensional systems. Throughout the quarter we have learned of the extreme utility of information—theoretical approach towards analyzing systems, largely due to its generality. If given a sequence of discrete measurements, the methods outlined throughout this course are able to determine patterns in the system, leading towards an optimal predictability of the system's future behavior. The question that this project's topic concerns is: what if we do not have a well—defined "sequence" of measurements? This would be a difficult endeavor if it was attempted in full generality. So I have focused, in particular, on two—dimensional patterns that arrive in a, still fairly general, spin system.

While a generic sequence of symbolic measurements occurs often in practice, say with numerical instrument readings (e.g. voltage, current, pressure, etc.), there are occasions when larger dimensionality is an important attribute of the system. I have already given an example of one. One—dimensional and two—dimensional Ising—spin systems can be solved analytically (the two—dimensional Ising system can only be solved analytically with no applied magnetic field). The two systems are decidedly different in both behavior and appearance. The one dimensional system exhibits no finite—temperature phase transition, while the two dimensional system does. Any given spin in a one—dimensional system will always have only one nearest—neighboring spin. In a two—dimensional system, the number of nearest—neighbors depends on the geometry of the system, leading to a number of different behaviors. In the triangular lattice, for example (a geometrically frustrated system) each spin has six nearest—neighbors and, unlike most two—dimensional geometries, in simple cases, has no finite—temperature phase transition.

The system I have studied is a two—dimensional spin system, on a square lattice with periodic boundary conditions, and with nearest—neighbor and next—nearest neighbor interactions. To model the system I have written a simple Monte Carlo simulation with a single—site Metropolis algorithm for controlling the spin dynamics. While I have employed the use of a fairly general spin system, I have limited myself to tractable parameter settings (simple enough to analyze) in my attempt to quantify the structure of the system. I have employed the use of mutual information formulation of the excess entropy (E_I) of the system. My goal, more explicitly stated, was simply to explore both the occurrence of structure in a $2D$ spin system and the utility of E_I in detecting it. More specifically, since the spin system model I am using is quite general, I have calculated the local excess entropy in the neighborhood around each lattice site. I will state now, that I had no previous expectations for uncovering any flaws in the formulation of this information—theoretical quantity or to goals of proving any grand mathematical properties. My purpose has, from the start, been merely to fulfill a curiosity as to the applicability of this structure—detection technique.

I attempted to look at two systems in particular: a system of spins with an inhomogeneous, external magnetic field, and a system of spins undergoing spin nucleation. The first of which, would have hopefully applied insight into the detection of large—scale structure inhomogeneous in space. The second was an attempt at to look at structure which was emerging and decaying in time. However, I did not allow for enough time to complete the project and even as this report is being read, my simulation is still likely running. I have reason to believe however, as I will address in the "Results" section, that only qualitative results could have been extracted from the simulation data, anyway.

Background:

$2D$ Structure[1]

Compared to $1D$ systems, $2D$ systems are inherently different. This is largely due to the lack of an obvious, implied ordering in which to read each symbol. The information—theoretical measure of generic structure (existence of patterns) in a system is the excess entropy. In $1D$ systems, the three formulations of the excess entropy (convergence, mutual information, subextensive):

$$\mathbf{E}_C = \sum_{L}^{\infty} [h_\mu(L) - h_\mu]$$

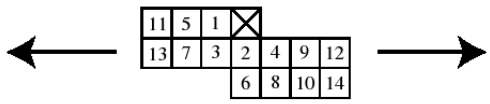
$$\mathbf{E}_I = I(\overleftarrow{S}; \overrightarrow{S})$$

$$\mathbf{E}_S = \lim_{L \to \infty} [H(L) - h_\mu L]$$

are all equivalent. This is not the case in two—dimensional systems. Because of this lack of a well—defined ordering, we must utilize different means of acquiring the statistics of the system, extending the area of observation into the second dimension. This is probably more clear when given in an example.

To compute E_C, we must compute the block entropy rate, h_μ. When a $1D$ system is stationary ($S_0 = S_t$, where S_0 is the set of observable symbols S at position 0 in the sequence of measurements received and S_t is the set of observable symbols t positions in the "future" direction), we can represent h_μ as the entropy of a target symbol (in my case, the lattice—site's spin value) conditioned on all observable symbols in the "past": $H(S_t|\overleftarrow{S})$. By the term "future" ("past"), I am referring to all the symbols observed to the right (left) along the one dimension. This is somewhat arbitrary, since, we could easily read the symbols from right to left; however, in either case, each spin is still bordered by its nearest neighbors.

As I have been saying, in $2D$ systems, there is no obvious analogy between the set of symbols that, in $1D$, we would call the "past" ("future") and any set of symbols in a $2D$ system the occur "before" ("after") the target site. There are now two dimensions into which these symbols extend. It is now necessary to record the probability of observed symbols in a two—dimensional block containing our target symbol location and the entropy of such a block has been shown to converge most quickly $[2, 3, 4, 5, 6, 7, 8]$ when considering a block geometry like so[1]:



The target symbol location is marked with an "X" and the numbering scheme is taken in order of increasing Euclidean distance to the target symbol location. Even with this use of increasing distance as a guideline for ordering our observed symbols, there is still ambiguity as to whether the symbol of distance, 1, to the left or below is recorded first, which elucidates my point about the lack of a well—defined ordering scheme. I also wish to highlight thickness of this semi—infinite strip of increasing block length. It has been shown that it is unnecessary to consider a thickness greater than the distance of interaction$[2, 3, 4, 5, 6]$. I will refer to this point, momentarily.

While this has been a useful point of discussion, I did not, however employ the convergent formulation of the excess entropy, E_C, as my tool for analyzing $2D$ structure. Feldman and Crutchfield[1] had already shown that, given a spin system with no greater than next—nearest neighbor interactions (as I have implemented), E_C does not capture all the structure present, while the mutual information formulation E_I, does. The reason for this is, apparently, in the means of acquiring the statistical quantities. With the range of parameters they observed, there was shown to be structure that was periodic over four lattice sites but with different geometries. E_C was unable to distinguish the difference between these different geometric structures while E_I was. E_I, as Feldman and Crutchfield employed it (as well as how I have employed it), was taken as the mutual information between two contiguous blocks of dimensions $4x2$ (*row x column*).

This larger contiguous block of observed symbol locations was apparently more effective at detecting different structures in their system. I admit, that since my point was to analyze inhomogeneous

$$\mathbf{E}_{\mathrm{I}} \equiv \lim_{M,N\to\infty} I\left[\ \overset{\longleftarrow M \longrightarrow}{\uparrow \atop N \atop \downarrow}\boxed{};\boxed{}\overset{\longleftarrow M \longrightarrow}{\uparrow \atop N \atop \downarrow}\ \right]$$

patterns, two different measures of structure would be a valuable comparison. It is, I deem, overly hopeful given the available amount of time but would perhaps be nice as a future endeavor. While Feldman and Crutchfield used both of these quantities (E_C E_I) to analyze their system I have attempted a local formulation of the E_I. That is, the probability of a particular pattern occurring within the two contiguous observed blocks which enters into the computation of the mutual information is acquired by recording future evolutions of the system's equilibrium state at each block location, individually (indexed by the upper left—hand corner of the combined $4x4$ block).

Before moving onto my particular system, I would like to say a few words about work done previously on spin systems, by Feldman and Crutchfield[1]. They, too, analyzed a two-dimensionaly Ising spin system and compared it to the standard means of detecting structure in spin systems, the structure factor:

$$S(p) = \sum_{r=1}^{\infty} \cos((2\pi r)/p)\Gamma(r),$$

$$\Gamma(r) \equiv \langle s_0 s_r \rangle - \langle s \rangle^2,$$

where $S(p)$ is the structure factor for periodicity p, $\Gamma(r)$ is the spin-spin correlation function which detects a correlation between spins horizontally or vertically at a distance r from the reference spin s_0. They showed that generality of the excess entropy quantities allows for periodicities of any period-length to be detected, while the more common structure factor must be computed for each period-length over which one expects to see structure. Furthermore, (as previously alluded to) different structural geometries given the (NN) and (NNN) Ising systems they analyzed are discernible using E_I, while they are not nearly so obvious using $S(p)$. The only drawback of the excess entropy in analysis of a spin system, I have already stated but in a different light. Depending on the desired outcome of the analysis, detection of structure at a particular periodicity may be desired. The excess entropy is sensitive to all periodicities, which, in most cases, is a plus, but this also means it not instructive as to the particular periodicity. However, the simple fact that the information-theoretical approach is generic enough to apply to all statistical systems means that it can be applied where the spin-spin correlation function and structure factor can not.

Dynamical System:

This leads me directly into the slight bit of necessary background for the particular system I have studied (the $2D$ spin system with nearest and next—nearest neighbor interactions and confined to a square lattice) and computational technique I employed (the Monte—Carlo simulation with a single—spin Metropolis algorithm).The Hamiltonian governing the energetics and dynamics of the system which I have used is given by:

$$\mathcal{H} = -\sum_{<ij,kl>nn} J^1_{ij,kl} S_{ij} S_{kl} - \sum_{<ij,kl>nnn} J^2_{ij,kl} S_{ij} S_{kl} - \sum_{ij} B_{ij} S_{ij},$$

where the first (second) summation ranges over NN (NNN) pairs of spins, $J^x_{ij,kl}$ are the coupling constants of the indexed pair of spins, $S_{ij} \in [-q, q]$, and B_{ij} is the magnetic field at the indexed

lattice site. The S_{ij} refer, in particular, to the $z-$component of the spin. In actuality, the interaction terms in the Hamiltonian should involve the dot product between the two spins in question, however I have chosen this simplification as a matter of tractability. Positive coupling constants indicates ferromagnetic interaction (i.e. parallel spin alignment), while negative coupling constants indicates an antiferromagnetic interaction (i.e. antiparallel alignment). The system, in general, will have spin interactions reaching to next—nearest neighbors and site—by—site control over both the coupling constants and the applied magnetic field. I will address the implementation of this system and how that governs the equations of motion in the following section.

Methods:

Since it relates to the dynamics of the system, I wish to say a bit about the Monte—Carlo simulation method as applied to a lattice of spins. The technique is extremely simple. The initial spin configuration of the system is random and the system is evolved by, with each iteration, randomly selecting a single spin making a computation of the energy difference between the current system and one where the selected spin is flipped to a new spin value. If the energy difference is negative, the flip is performed. If the difference is positive, the thermal energy of the system may still be sufficient to flip the spin to its new value. The probability that the spin will be thermally excited is given by the Boltzmann factor:

$$Prob \propto \exp(-\Delta E/k_B T)$$

where ΔE is the energy difference between the current state and the "flipped—spin" state, k_B is the Boltzmann constant and T is the temperature. This quantity for positive ΔE, will always be between 0 and 1. A comparison is, thus, made between the Boltzmann factor and a randomly generated number between 0 and 1. If the Boltzmann factor is greater than this random number, the spin is flipped to its new location, if lesser, the spin remains unchanged. As I have implemented the program, a spin can take on a range of values, thus, the final spin state is selected at random, as well. Thus, this system has both deterministic properties ($\Delta E < 0$) and statistical properties (Boltzmann factor, thermal effects).

Evolving the spin system using the Monte—Carlo simulation was only a small part of the project. Far more energy was expended in extracting the statistical properties from the system. As the spin system evolves, it is first necessary to scan through the lattice and acquire the spin configuration. In particular, I found the mutual information between two 4x2 contiguous blocks of spins. To do so, I established an arbitrary ordering in which to label the spins within the spin blocks and, based on the shifted value of the spin $S_{ij} \in [0, 2q]$ and its "order" within the block, converted the pattern value as a base $(2q+1)$ number to base 10. (This is analogous to the ordering of rules in cellular automaton models, with a binary system $S_{ij} \in (0, 1)$.) Once the system has finished evolving and the patterns have been collected, each unique pattern for each block (including the joint, 4x4, block) must be extracted and its probability of occurrence determined. For homogeneous parameter settings ($J^1_{ij,kl} = J^{(NN)}_{ij,kl} = J^1$, $J^2_{ij,kl} = J^{(NNN)}_{ij,kl} = J^2$, and $B_{ij} = B$), one is able to find the probability that a pattern will occur anywhere, globally, on the lattice. If parameter settings are inhomogeneous, only patterns that occur locally on the lattice are compiled together. Once the pattern probabilities are known for the lefthand, righthand, and joint blocks, determining E_I, is simple:

$$\mathbf{E}_I = \mathbf{I}(S^L; S^R)$$

$$\mathbf{I}(S^L; S^R) = \sum_{s^L} \sum_{s^R} p(s^L, s^R) \log_2[p(s^L, s^R)/p(s^L)p(s^R)],$$

where $s^{L,R}$ is the pattern number of the spin configuration in the left/right blocks, and each sum ranges over all possible spin configurations within each block.

Despite the generality of the spin system and, thus, the potential for finding interesting two-dimensional structure, the program I had written also included long run-times ($\sim$ 11 to 23hrs, depending on whether local E_I, global E_I or both, were computed). I, therefore, only had time to look at two systems. The time scale of the systems I selected were dependent on the lattice size. One time scale was equivalent to the number of iterations it took to flip each spin twice, *if* every spin was to be flipped an equal number of times. The first was a 48x48 lattice system with antiferromagnetic coupling between both nearest ane next—nearest neighbors ($J^1 = J^2 = -4$). The magnetic field in the system was zero at most locations, however, strong magnetic fields were placed with slightly irregular intervals in groups of 4x3 or 4x4 lattice sites. The system was equilibrated over $\sim$ 2x10^5 time scales and then 1000 measurements were taken every 20 time scales. The physical analogy of such a system would be a crude representation of the effect of vortices in a Type−II superconductor on the localized magnetic moments within the material. The vortices of a superconductor are magnetic flux quanta which permeate the material in localized places. The core of the vortex is where the superconducting order parameter goes to zero, and has a is of finite diameter. Physically, this is where the energy of circulation of the Cooper pairs is on the order of that necessary to "de-pair" the electrons.

Finally, I also attempted to apply an adapation of this method to the phenomenon of spin nucleation. A 100x100 site, spin system was held under a strong, homogeneous magnetic field during the equilibration phase ($\sim$ 2x10^5 timescales). Upon equilibration, the magnetic field is flipped and the spins follow suit. The structure in this system changes as it is evolved in time and, thus we cannot lump together further iterations when we extract the probability of spin configuration occurrence. Bins in iteration time must be established and, in the manner which I attempted, the global E_I within each bin computed for comparison to the particular spin configurations. The goal in this case, is not to see merely the emergence of structure, but also the decay of structure as the spins become completely parallel with each other.

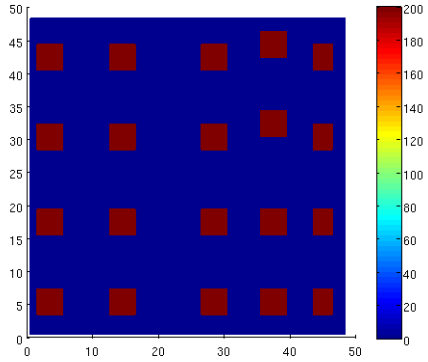
Results

This section will unfortunately be far shorted than I had expected when setting out on this project. On first blush, the detection of interesting structures that emerge in a highly generic two-dimensional spin system seemed a weighty undertaking but I managed to narrow down my avenue of approach. I did so, however, a bit too late. As of this moment, my simulations have *still* yet to finish running. As I will soon explain, I believe that equilibration time for my Monte—Carlo simulation is longer than I accounted for. It seems that with the long run-times that my simulation carries with it, I am forced to comment primarily on my attempts, and the particulars of my failures.

Inhomogeneous $\overrightarrow{B}$ System

The magnetic field of this system is shown below:

External inhomogeneous magnetic field



There were two interesting features of this system which I wished to address. The system contains both a large scale structure to it, and slight inhomogeneity as to its periodicity. I had been curious to see what happened at the boundaries of these regions of high magnetic field. Now, however, I am left pondering a different question because, even if my simulation had completed, I realize it would not adequately characterize the structure of this sytem. Despite this being a very simple system, the structure of the system is on a scale larger than the area of observation I used to investigate it. I had already mentioned that I only used a 4x4 block of contiguous spins to calculate the mutual information (between the two 4x2 blocks comprising the larger). I am left, therefore, wondering how large scale structure would manifest itself when viewed on a smaller scale. Perhaps the fact that a local E_I estimate was attempted could have accommodated for the lack of foresight as to the structure of the system, i.e. different excess entropy readings would occur at different relative positions with respect to the high $\overrightarrow{B}$ region. But, this would likely provide little more insight into the system than simply looking at a picture of the magnetic field, as seen in the figure above. This, it seems, can be used as a lesson in the scale at which we investigate structure. Even though the interaction distance of this system was no larger than between next—nearest neighbors and thus the area of investigation would not normally need to exceed this size, the inhomogeneity of the applied $\overrightarrow{B}$ called for significantly larger area of observation. Here also, is where the most insight could have been gained through a comparison between the mutual information and convergent formulations of the excess entropy quantity, since the geometric structures differ between the two.

Spin Nucleation

The idea of the emergence and decay of structure in a system of nucleating spin-islands, I found very interesting. Unlike the previous sytem, this has a degree of randomness in the large—scale structure. Unlike the previous system, the parameter settings on it are completely homogeneous and the anticipated development of islands would not be as a result of any preferential position within the lattice. Because of this, I attempted a global E_I estimate of the system. With little else on which to comment, I would like to preface the fact that, had the simulation for the global E_I estimate of this sytem completed, because of a possible oversight on my part, it would have (I believe) been incorrect regardless.

Comparison and Calibration

This is a necessary topic of discussion for it relates to the interpretation of my results. I compared my program to the a few J^1 values between the strongly ferromagnetic regime ($J^1 > 0$, $J^2 < 0$,

$|J^1| \ll |J^2|$) and next-nearest neighbor antiferromagnetic regime ($J^1 = 0$, $J^2 < 0$) analyzed by Feldman and Crutchfield[1] (the $J_1 \geq 0$ region of the $\mathbf{E}_I$ vs. J_1 graphs). In the case of the strongly ferromagnetic parameters I found excellent agreement with both local and global E_I.

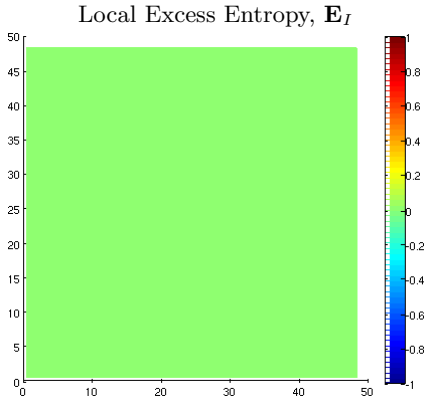


Figure 1: spin,$q = .5$; $J^1 = 12$; $J^2 = -4$; $B = 0$: ferromagnetic range. See text for further discussion

Though this figure is a rather boring, it is supposed to be. When the system is in the ferromagnetic state, all spins are aligned parallel to each other. With parallel alignment there is no spatial information stored within the spin configurations and, thus, the excess entropy is zero. If the system is homogeneous, any structure found within the local excess entropy will be reflected in the global. I should insert the caviat, that this is true if the structure within the entire system is smaller than the area of observation used to inspect it. This is for the same reason that the convergent excess entropy only requires a block thickness just larger than the interaction distance (as previously mentioned).

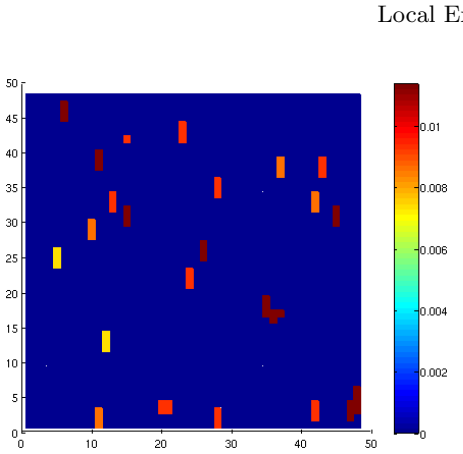


Figure 2: $J^1 = 1.2$,$J^2 = -4$,$B = 0$

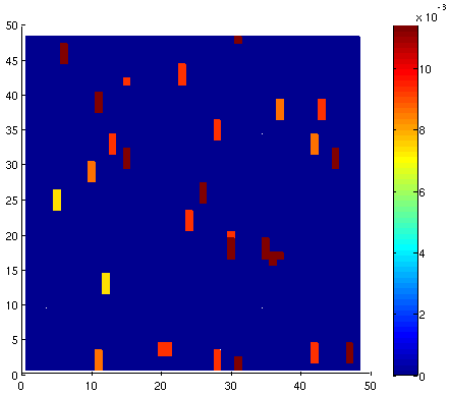


Figure 3: $J^1 = 0$,$J^2 = -4$,$B = 0$

Though as a ferromagnet, my program yields what's expected, that is not the case outside of this regime. I wish to, at least, point the possible causes of error in my simulation technique. First of all, looking at Figures 2 and 3, above, structure appears to be forming in both of these systems but, referring to $J^1 \approx 0$ region in Feldman and Crutchfield's paper, I should expect a ground state has formed with $E_I =$ either 2 or 3 *bits*. Judging from the appearance of the two non-ferromagnetic

local E_I graphs, it seems that the system may not have had sufficient time to equilibrate to one of these ground states. In theory, if the system has not equilibrated, I should so both an incorrect local and global E_I. Let us keep this in mind.

One alternate explanation is that the technique did not compute the block probabilities correctly. This may be correct with the global E_I (which I address in a moment), but in the both cases, I did check that the sum of all observed patterns' probabilities within each block was equal to one. At least that much can be said about the simulation. Another possible reason for the discrepancy is that, by acquiring a comparable number of samples to the simulation done by Feldman and Crutchfield, I only achieve fair enough statistics when computing the global excess entropy (as they have done), while the local excess entropy had a fair amount of statistical error. If this was the only explanation, however, I would achieve a poor estimate of the local E_I and a fair estimate of the global E_I. It is quite clear that my local excess entropy estimate for the two systems above in **??** and **??**, but as are my estimates of the global E_I: both $\approx 1(bit)$.

My final attempt at explaining these discrepencies lies in my combination of local statistics in achieving the global E_I. When accumulating spin configuration patterns, I did so within a particular block and, to find the global probabilities of pattern occurrence I combined the list of patterns accumulated from *every* block into a master list and counted like patterns. The block patterns themselves were overlapping. This may seem, at first, to be a mistake however it is perfectly analogous to the one—dimensional system. When acquiring word probabilities of varying lengths in a $1D$ system, we do look at overlapping word distributions as creating unique words. This is due to our lack of knowledge as to a unique starting symbol. Simply extending this method into two dimensions, overlapping blocks should be counted as unique block spin distributions. I, therefore, deem that this is not the problem. Having addressed these issues, the only conceivable conclusion, in my mind, is a result of poor equilibration time.

Conclusion

It seems that the majority of my conclusions must be drawn from the failure of my attempts, rather than any kind of insight into my results (since they do not, exactly, exist). There is a necessity, it seems from the discussion of the inhomogeneous magnetic field system, to select multiple geometries and scales in the detection of structure in a two—dimensional system. The effects of geometry do not occur in a $1D$ system. This is the benefit of multiple formulations of the excess entropy, that we have the means of detecting generic structure in a system. Had I allowed for more time to investigate the matter, I most certainly could have looked in more depth at the effects of these different geometries but that is, alas, not the case.

Appendix: Program Annotations

`montespin.m`

This is the primary, master program, containing all other functions below. In this, the system is evolved using the single-spin Metropolis algorithm, the statistics are acquired, and the information-theoretical quantities are computed.

`flips.m`

Computes the energy of the system and, if it is energetically or probablistically favorable, flips the randomly selected spin to the randomly selected final spin position. The selection of the spin and its final value are actually computed in "montespin.m" and the final spin value is not allowed to duplicated the current value.

`pattbbf.m`

Acquires the spin configuration patterns within each block of observation.

`probblksf.m`
`lcleeinfof.m`

Acquires the local statistical information from "pattbb.m" and computes the local E_I.

`probglobf.m`
`eeinfof.m`
`probglobf07.m`
`eeinfof07.m`

Acquires global statistical information from "pattbb.m" and computes the global E_I. The last two compute the global E_I, but binned by iteration number for use with the spin nucleation simulation.

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