For a system defined with many possible configurations defined through a model Hamiltonian, calculated from model potentials, or through first principles methods it may be desirable to calculate the density of energy states $G(E_j)$. With the energy density of states the partition function,

$$Z = \sum_i^{\Omega} e^{\frac{-e_i}{k_B T}} = \sum_j^{\Pi} G(E_j) e^{\frac{-E_j}{k_B T}} , \qquad (1)$$

can be exactly calculated an from it many important properties of interest determined. Properties of interest calculated from the partition function include free energy, entropy, specific hear, and ensemble averages. One method of solving this problem has been temperature dependent simulations involving Metropolis algorithm and histogram re weighting techniques[1]. Another algorithm called the Wang and Landau algorithm[2] has been developed which is temperature independent. In this paper a method is proposed that combines the use of random sets along with the importance sampling method of the Wang and Landau algorithm. This algorithm is referred to as the "B$_L$ENDER" (B$_L$end Each New Density Each Round) algorithm. The name "B$_L$ENDER" functions as an acronym and adjective which comes in part because how it blends the ideas of a random set and the Wang and Landau method, and also due to the nature of the algorithm iteratively blending histograms to produce a converged density of states. The purpose of developing the "B$_L$ENDER" algorithm was to work towards an algorithm that is both accurate and trivial to parallelize. The Wang and Landau method does have parallel versions, including restricting random walkers to specific energy ranges or allowing the walkers to explore the entire space while periodically communicating with each other [3, 4, 5]. The "B$_L$ENDER" is trivial to parallelize as it is based on a set of random walkers than each can explore the entire energy range. It is hoped that due to the "B$_L$ENDER" being presented in the form of sets that the mathematics of set theory and real analysis can be used to analyze the algorithm and possibly further extended its capabilities from those presented in this work.

In a previous paper the notion of the master set $\{\Sigma_i, e_i\}_\Omega$ of the Ω total configurations and energies was put forth. The master set refers to the actual configurations of the defined system. In practice to calculate the density of energy states $G(E_j)$ may be possible through randomly sampling the configurations space. In a previous work it was shown that a properly scaled histogram of a sampled set $\{\Sigma_s, e_s\}_\mathcal{S}$ converges to the exact density of states $G(E_j)$ as the the number of samples $\mathcal{S}$ goes to infinity. The problem with this method is that if Ω is large, which it is for many problems, then the computationally effort to achieve convergence is not feasible. This work tackles this issue produce an algorithm that is highly parallel in terms of the calculations of the energies but also incorporates importance sampling such as in the Wang and Landau method.

The "B$_L$ENDER" algorithm proposed in this work is given as follows. It is noted that the following algorithm is in terms of producing a relative density of states $H(E_j)$.

1. $H(E_j)^i, \ \{\Sigma_s, e_s\}_\mathcal{S}^i$

2. $\{\Sigma_s, e_s\}_\mathcal{S}^i \rightarrow \{\Sigma_s^{'}, e_s^{'}\}_\mathcal{S}^i$

3. $H(E_j)^{Ii} = H(E_j)^i + \mathcal{H}(E_j, \{e_s^{'}\}_\mathcal{S})$

4. $\Sigma_s^{i'} \rightarrow \Sigma_s^{i+1}, \ P(1, H(e_s)^{Ii}/H(e_s^{'})^{Ii})$
   $else \ \Sigma_s^i \rightarrow \Sigma_s^{i+1}$

5. $H(E_j)^{i+1} = H(E_j)^i + C_o \mathcal{H}(E_j, \{e_s\}_\mathcal{S}^{i+1}) \dfrac{H(E_j)^{Ii}}{\sum_j H(E_j)^{Ii}}$
   $$(2)$$

Where $H(E_j)^0 \equiv \mathcal{H}(E_j, \{e_s\}_\mathcal{S}^0)$ with $\mathcal{H}(E_j, \{e_s\}_\mathcal{S})$ being a histogram function that counts the number of energies E_j in the set $\{e_s\}_\mathcal{S}$. In this work $\{\Sigma_s, e_s\}_\mathcal{S}^0$ are a randomly(uniformly) drawn set from the configuration space $\{\Sigma_i, e_i\}_\Omega$. In the second step a random change is applied to each element of the sampled set $\{\Sigma_s, e_s\}_\mathcal{S}^i$ to produced a "perturbed" set $\{\Sigma_s^{'}, e_s^{'}\}_\mathcal{S}^i$, for the Ising model this could be randomly flipping a spin. In the third step a histogram of the "perturbed" set is added to the current estimate of the density of states $H(E_j)^i$ to produce an intermediary density of states $H(E_j)^{Ii}$. In the fourth step a random number is drawn between zero and one for every sampled configuration, if this number is less then the

1

ratio of the density of states $H(e_s)^{Ii}/H(e_s^{'})^{Ii}$ then the perturbed configuration $\Sigma_s^{'i}$ goes to Σ_s^{i+1}, else the unperturbed configuration Σ_s^i goes to Σ_s^{i+1}. In the fifth step a histogram of the updated $\{e_s\}^{i+1}$ energies is made and added (blended) in to the current density of states $H(E_j)^i$ by multiplying by a constant(which effects convergence) and the relative probability of each energy E_j in the the intermediary density of states $H(E_j)^{Ii}$. After the algorithm is deemed to be complete it is necessary to re-normalize the iterated relative density of states $H(E_j)^f$ at the final iteration f as follows,

$$
\begin{aligned}
&1.\ A = \sum_j H(E_j)^f \\
&2.\ G(E_j) \approx H(E_j)^f \frac{\Omega}{A} ,
\end{aligned}
\tag{3}
$$

to produce the properly normalized estimated value of $G(E_j)$.

In this work the algorithm discussed is tested using the 2-d zero field ferromagnetic Ising model. The total energy of a square 2-d Ising model of dimension $n \times n$ with periodic boundary conditions is given by,

$$
e_i = -J \sum_{k,l=1}^n \sigma_{k,l}^i \left(\sigma_{k+1,l}^i + \sigma_{k,l+1}^i \right) .
\tag{4}
$$

Where e_i denotes the i'th energy of the set $\{\Sigma_i, e_i\}_\Omega$ configurations and energies. The configurations and energies of the 2-d Ising model are inherently defined by the lattice site spin variables $\sigma_{k,l}^i$ and coupling constant J. In this work $J = 1$. Several tests of the algorithm will be performed. A test of the convergence properties with respect to the number of samples $\mathcal{S}$. A test of the convergence properties in terms of the size of the system determined by n. These test will utilize comparisons to the exact results. Also a qualitative understanding of the convergence as a function of time will be presented. The first test is a test to show the convergence of the algorithm in terms of the number of samples $\mathcal{S}$ and the number of iterations of the algorithm. To test the accuracy of the simulations the results will be compared to the exact result solved by Beale [6]. The accuracy of the

simulation will be determined by,

$$
\epsilon(I, o) = \frac{1}{\Pi} \sum_{j=1}^{\Pi} \frac{|\ln(G_{ex}(E_j)) - \ln(G_{bl}(E_j, I, o))|}{\ln(G_{ex}(E_j))} .
\tag{5}
$$

Where $G_{ex}(E_j)$ is the exact density of states, $G_{bl}(E_j, I, o)$ is the density of states at iteration number I from initial conditions and trajectory o. To test the convergence in terms of number of samples $\mathcal{S}$ and number of iterations I for $n = 12$. The simulations where done until iteration average,

$$
\mathcal{E}(I) \equiv \langle\, \epsilon(I, o)\, \rangle_{I'} = \frac{1}{I} \int_0^I \epsilon(I', o) dI' ,
\tag{6}
$$

was less then 1%, the corresponding number of iterations was recorded, this was then repeated for multiple simulations. The average value of I over initial configurations and trajectories that produced a specific value of $\mathcal{E} = c$ equal was then calculated to give,

$$
\mathcal{I}(\mathcal{E} = c) \equiv \langle\, I(\mathcal{E} = c)\, \rangle_o .
\tag{7}
$$

It is noted that the error is only well defined when all of the possible energies have been located. Correspondingly we can define an $\mathcal{I}(\mathcal{E} \,!= \infty)$ such that what is meant is the average iterations to find all of the energies. In Fig 1(a) it is shown how the number of iterations needed to achieve $\mathcal{E} = 1\%$ scales with the number of samples for a 12×12 system, for visual purposes the x-axis is on a natural log scale. Another interesting scaling property is the number of iterations necessary to find all of the energies in the system, this is shown in Fig 1(b).

Is is hypothesized that the average iterations $\mathcal{I}$ in both Fig 1 (a) and (b) are of the exponential form,
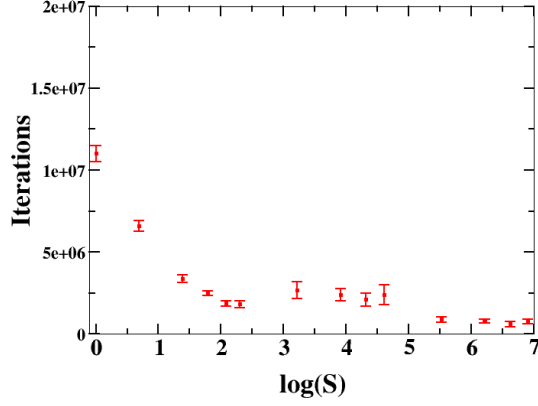
$$
\mathcal{I}(\mathcal{S}) = \mathcal{I}_o (1 - Ce^{-\frac{\lambda}{\mathcal{S}-1}}); .
\tag{8}
$$

Where C and λ are to be determined constants and $\mathcal{I}_o$ is $\mathcal{I}(\mathcal{S} = 1)$. This equation implies,

$$
(\mathcal{S} - 1) \ln(-\mathcal{I} + \mathcal{I}_o) = (\mathcal{S} - 1) \ln(\mathcal{I}_o C) - \lambda .
\tag{9}
$$

is linear. In Fig plots using the mathematical operation of the left hand side of Eq 9 on the data from Fig 1 (a) and (b) for $\mathcal{S} > 1$ are shown. These plots
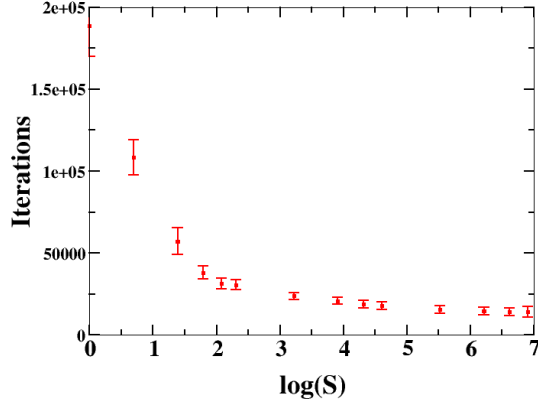
(a)

(b)

Figure 1: (a) average number of iterations($\mathcal{I}$) necessary to achieve $\mathcal{E} = 1\%$ and (b) average number of iterations($\mathcal{I}$) necessary to find all of the energies. Each for a for a 12X12 system.

demonstrate that Eq 8 is a good approximation to the scaling. So although it appears the scaling in terms of number of iterations(Wall Time) to achieve a certain accuracy is limited by the exponential decay there is a linear regime where the speed up is approximately proportional to the number of samples. It is hypoth-

esized that this scaling behavior will be of the same form given by Eq 8 for different system sizes but will different values for the characteristic constants C and λ.
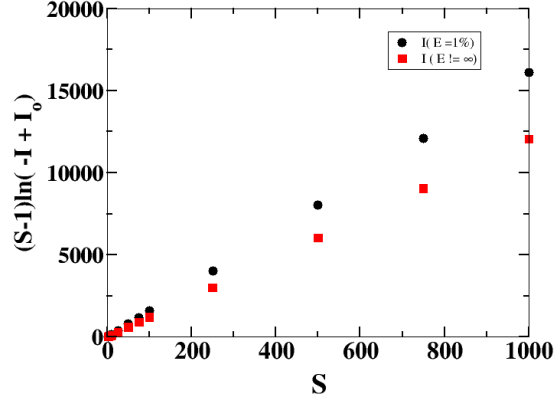

Figure 2: $(\mathcal{S}-1)\ln(-\mathcal{I}+\mathcal{I}_o)$ for the average iterations to reach 1% error (black circles) and for the average iterations to find all of the energies (red squares).

Another aspect of the algorithm to consider is the scaling of the number of average number of iterations $\mathcal{I}(\mathcal{E} = c)$ and $\mathcal{I}(\mathcal{E}! = \infty)$ as a function of system size. In Fig 3 the average number of iterations is shown vs the log of the number of configurations Ω. In Fig 3 it appears that the number of iterations to reach $\mathcal{E} = 1\%$ scales linearly with $\ln(\Omega)$. Considering $\Omega = 2^{N^2}$ for the 2d Ising model and that one Monte Carlo time step defined as $MC \equiv \frac{I}{N^2-1}$ ($N^2 - 1$ is the number of energies E_j) the number of MC for this algorithm appears to be a constant given by the slope of Fig 3. Overall the tests of the algorithm are encouraging for its use and demonstrate it is a viable method for accurate calculation of the energy density of states. From this many important thermodynamic properties can be determined but it may be considered a draw back that ensemble averages of a general order parameter $a_i \equiv a(\Sigma_i)$. Altough not implemented in this work it may be possible to acheive
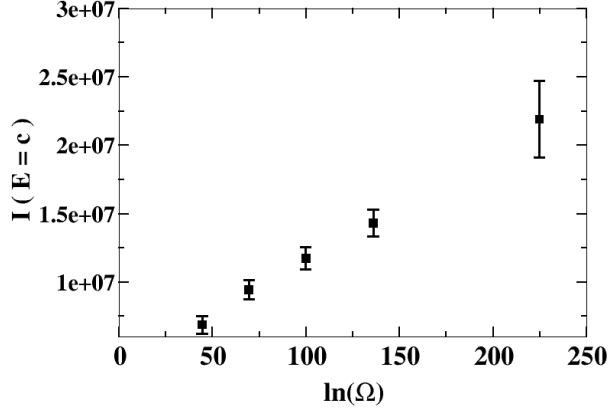
Figure 3: Average number of iterations to reach $\mathcal{E} = 1\%$ vs $\ln(\Omega)$ for $\mathcal{S} = 1$. Going from left to right each point corresponds to N= 8, 10 ,12 , and 18 respectively for the N×N models.

this considering the following equation,

$$\langle a \rangle = \sum_{i}^{\Omega} a_i \frac{e^{-\frac{e_i}{K_b T}}}{Z} =$$
$$\sum_{j}^{\Pi} < a_i >_j G(E_j) \frac{e^{-\frac{E_J}{K_b T}}}{Z} \ . \tag{10}$$

Where $< a_i >_j$ is the average of a_i over all configurations with energy E_j. So if a running average of the visited values was made during the simulation then it may be possible to approximate ensemble averaged order parameters over the entire temperature range.

References

[1] David P. Landau and Kurt Binder. *A Guide to Monte Carlo Simulations in Physics*. Cambridge University Press, fourth edition edition, 2015.

[2] Fugao Wang and D. P. Landau. Efficient, multiple-range random walk algorithm to calculate the density of states. *Phys. Rev. Lett.*, 86:2050–2053, Mar 2001.

[3] Junqi Yin and D.P. Landau. Massively parallel wanglandau sampling on multiple gpus. *Computer Physics Communications*, 183(8):1568 – 1573, 2012.

[4] Lixin Zhan. A parallel implementation of the wanglandau algorithm. *Computer Physics Communications*, 179(5):339 – 344, 2008.

[5] Thomas Vogel, Ying Wai Li, Thomas Wst, and D Landau. Generic, hierarchical framework for massively parallel wang-landau sampling. 110:210603, 05 2013.

[6] Paul D. Beale. Exact distribution of energies in the two-dimensional ising model. *Phys. Rev. Lett.*, 76:78–81, Jan 1996.