Abstract. We will describe our developments leading to an automated workflow approach that will utilize machine learning methods to combine first principles density functional theory (DFT) calculations with classical Monte-Carlo (MC) simulations. This method allows the investigation of the statistical mechanics and the finite temperature behavior of real materials with complex compositions and interactions of their constituents. The investigation of finite temperature properties using MC methods requires a large number of evaluations of the system’s Hamiltonian to sample the phase space needed to obtain physical observables as function of temperature. DFT calculations can provide accurate evaluations of the energies, but they are too computationally expensive for routine simulations. We demonstrate a solution to this problem that harnesses the computational power of large massively parallel computers by combining classical MC calculations with our first principles multiple scattering electronic structure code (LSMS), which shows exceptional scaling on current HPC architectures such as Summit, by employing Machine Learning (ML) techniques. This workflow that can consider both classical interaction models and artificial neural network based models, allows us to investigate alloy ordering transitions for increased simulation cell sizes. We investigate the behavior of different models, with respect to their training capability as a function of the data set size while avoiding the danger of overfitting the model. An important aspect of our workflow is the periodic retraining with newly generated first principles data based on the progressive exploration of the system’s phase space by the MC simulation. We will present results of these different approaches for training surrogate models for magnetic alloy materials.
1 Introduction

The investigation of finite temperature properties using Monte-Carlo (MC) methods requires a large number of evaluations of the system’s Hamiltonian to sample the phase space needed to obtain physical observables as function of temperature. Density functional calculations can provide accurate evaluations of the energies, but they are too computationally expensive for routine simulations. Surrogate models can alleviate the computational cost to complete classical MC simulations [18, 20, 27, 33, 36] since they can estimate finite temperature properties orders of magnitude faster than the original density functional theory (DFT) code. Although surrogate models generally do not attain the same accuracy as the physics-based model on which they are trained, a hybrid approach that combines initial inexpensive surrogate model evaluations with limited expensive DFT refinements can drastically reduce the computational time without significantly affecting the accuracy of the final inference with respect to running the DFT code throughout the entire classical MC workflow [29].

To this end, the identification of an appropriate surrogate model must take into consideration multiple factors such as (i) the dimensionality of the data space that needs to be explored, (ii) the amount of training data available, (iii) the complexity of the cause/effect relation that connects input features and target properties, (iv) the available computational resources. In situations similar to the ones addressed in this work where the training data is generated by running DFT calculations, (ii) and (iv) are strongly connected, as the computational resources available determine the amount of DFT data that can be generated for training.

Deep learning (DL) models have attracted a lot of attention in the material science community due to their ability to capture highly non-linear relations between input features and target properties [3, 6, 12, 20, 21, 24, 38]. However, their success relies on the subtle connection between the complexity of the DL model and the amount of available training data.

Here we will investigate the capability of two different classes of surrogate models to describe the energy of a magnetic alloy system with sufficient accuracy to be able to perform statistical mechanics investigations of alloy ordering.

In this paper we will first describe the two models we will be investigating, followed by a description of the physical alloy system, body-centered tetragonal FePt, that will provide the basis for our comparison. This will be followed by the results of our numerical experiments and finally we will discuss the results and conclude.

2 Surrogate models

2.1 Linear model

To model the energy of a refractory high entropy alloy system, the effective pair interactions (EPI) [19] was proposed. The energy is approximated by the
summation of local energies as follows,

\[ E \approx N \sum_{p' < p, m} V_{pp'}^{p'} \Pi_{p'}^{p} + V_{0}^{i} + V^{0} + \epsilon, \]  

(1)

where \( N \) is the total number of atoms, \( V^{0} \) is the bias term same for all sites, \( V_{0}^{i} \) is a single-site term depending only on the chemical component \( p \) of atom \( i \), and \( \Pi_{p'}^{p} \) is the proportion of \( pp' \) interaction in the \( m \)-th neighboring shell. The EPI model has been shown \[19\] to work well for non-magnetic alloy systems.

### 2.2 Graph convolutional neural network

GCNN models directly input atomic structure and converts it into a graph, where atoms are interpreted as nodes and interatomic bonds are interpreted as edges, and outputs total (graph-level) and atomic (node-level) physical properties. The architecture of a GCNN model is characterized by two sets of layers: the first set of layers learn features that are common to all the material properties and the last set of layers are separated into multiple heads to learn features that are specific to each material property, shown schematically in Figure 1. The shared graph convolutional layers are used to extract common relevant features from pairwise neighbor interactions and, through multiple layers, also represent many-body interactions. The following separate layers are fully connected and learn mappings between extracted features and the physical properties of interest.

![HydraGNN architecture](image)

**Fig. 1.** HydraGNN architecture when used as a surrogate model for DFT calculations of mixing enthalpy, atomic charge transfer, and atomic magnetic moment.

Our implementation of GCNN, called HydraGNN, uses Pytorch \[1, 28\] as both a robust NN library, as well as a performance portability layer for running on multiple hardware architectures. This enables HydraGNN to run on CPUs and GPUs, from laptops to supercomputers, including ORNL’s Summit and
NERSC’s Perlmutter. The Pytorch Geometric library built on Pytorch is particularly important for our work and enables many GCNN models to be used interchangeably. HydraGNN is openly available on GitHub.

2.3 Graph convolutional layers

A graph $G$ is usually represented in mathematical terms as

$$G = (V, E)$$

where $V$ represents the set of nodes and $E$ represents the set of edges between these nodes. An edge $(u, v) \in E$ connects nodes $u$ and $v$, where $u, v \in V$, $E \in V \times V$. The topology of a graph can be described through the adjacency matrix, $A$, an $N \times N$ square matrix where $N$ is the number of nodes in the graph, whose entries are associated with edges of the graph according to the following rule:

$$A[u, v] = 1 \text{ iff } (u, v) \in E$$
$$A[u, v] = 0 \text{ otherwise.}$$

The degree of a node $u \in V$ is defined as:

$$d_u = \sum_{v \in V} A[u, v]$$

and represents the number of edges connected to a node. Every node $u$ is represented by a $a$-dimensional feature vector $x \in \mathbb{R}^a$ containing the embedded nodal properties and also a label vector $y \in \mathbb{R}^b$ in tasks related to node-level predictions. In order to take advantage of the topology of the graph, many DL models include both the number of neighbors per node, as well as the length of each edge between nodes.

GCNNs embed the interactions between nodes without increasing the size of the input by representing the local interaction zone as a hyperparameter that cuts-off the interaction of a node with all the other nodes outside a prescribed local neighborhood. This is identical to the approximation made by many atomic simulation methods, including the LSMS-3 code used to generate the DFT training data, which ignore interactions outside a given cutoff range. GCNNs are DL models based on a message-passing framework, a procedure that combines the knowledge from neighboring nodes, which in our applications maps directly to the interactions of an atom with its neighbors.

The typical GCNN architecture is characterized by three different types of hidden layers: graph convolutional layers, graph pooling layers, and fully connected layers. The convolutional layers represent the central part of the architecture and their functionality is to transfer feature information between adjacent nodes (in this case atoms) iteratively. In the $k$th convolutional layer ($k = 0, 1, \ldots, K$), message passing is performed in sequential with the following operations:
1. Aggregate information from neighbors: the node $u$ collects the hidden embedded features of its neighbors $N(u)$ as well as the information on the edges (if available) via an aggregation function:

$$h^{k+1}_{N(u)} = \text{AGGREGATE} \left( m^k_v, \forall v \in N(u) \right),$$

where $m^k_v = \text{MESSAGE} (h^k_v, h^k_{e_{uv}})$ is a message obtained from neighboring node $v$ and the edge $e_{uv}$ that connects them. The vector $h^k_v$ ($h^k_v \in \mathbb{R}^{p_k}$) is the embedded hidden feature vector of node $v$ in the $k$th convolutional layer. When $k = 0$, the hidden feature vector is the input feature vector, $h^0_v = x$.

2. Update hidden state information: with $h^{k+1}_{N(u)}$ collected, the nodal feature of node $u$ is updated as in:

$$h^{k+1}_u = \text{UPDATE} \left( h^k_u, h^{k+1}_{N(u)} \right)$$

where UPDATE is a differentiable function which combines aggregated messages $h^{k+1}_{N(u)}$ from neighbors of node $u$ with its nodal features $h^k_u$ from the previous layer $k$.

Through consecutive steps of message passing, the graph nodes gather information from nodes that are further and further away. The type of information passed through a graph structure can be either related to the topology of the graph or features assigned to the nodes. An example of a topological information is the node degree, whereas an example of nodal feature in the context of this work is the proton number of the atom. A variety of GCNNs, e.g., principal neighborhood aggregation (PNA) [4], crystal GCNN (CGCNN) [38] and GraphSAGE [13], have been developed, differing in the definitions of functions AGGREGATE, MESSAGE, UPDATE for message passing. One simple example of the function combination is:

$$h^{k+1}_{N(u)} = W^{(k+1)}_{\text{neighborhood}} \sum_{v \in N(u)} h^k_v + b^k,$$

$$h^{k+1}_u = \sigma \left( W^{(k+1)}_{\text{self}} h^k_u + h^{k+1}_{N(u)} \right),$$

where $W^{(k+1)}_{\text{self}}, W^{(k+1)}_{\text{neighborhood}} \in \mathbb{R}^{p_{k+1} \times p_k}$ are the weights of $(k + 1)$th layer of GCNN and $\sigma$ is an activation function (e.g., ReLU) that introduces nonlinearity to the model.

PNA is used in this work and is one of the convolutional layers available in HydraGNN through Pytorch Geometric; PNA combines multiple aggregating techniques to reduce the risk of classifying two different graphs as identical. Batch normalizations are performed between consecutive convolutional layers along with a ReLU activation function. Graph pooling layers are connected to the end of the convolution-batch normalization stack to gather feature information from the entire graph. Global pooling layers aim at collapsing the node feature associated with each atom across a graph into a single feature. This is achieved by summing the local interactions of each atom with its neighbors and use the
result to estimate global properties. For atom (node) level features such as the atomic charge transfer and atomic magnetic moment, collapsing the information from all atoms into a total system feature is not needed. Fully connected (FC) layers are positioned at the end of the architecture to take the results of pooling, i.e. extracted features, and provide the output prediction.

Larger sizes of the local neighborhood lead to a higher computational cost to train the HydraGNN model, as the number of regression coefficients to train at each hidden convolutional layer increases proportional to the number of neighbors. Further details on the behavior of HydraGNN with different sizes of the local neighborhood have been previously reported [21].

3 Ferromagnetic materials

Itinerant ferromagnetic materials are typically metals. They exhibit magnetization even in the absence of a magnetic field. FePt is one of the examples of such a ferromagnetic material. The magnetic properties of this material are highly dependent on the chemical ordering and stoichiometry[33], according to which the magnetic state can change from ferromagnetic to antiferromagnetic[8], a non-collinear spin structure[14], or a mixture of antiferromagnetic orderings[34]. The total magnetic moment of FePt is presented in Figure 3. While pure Fe is magnetic and Pt is non-magnetic, the formation of magnetic moments in alloys is driven by the collective behavior of electrons in the alloy. Indeed there is a long history of trying to understand and describe the magnetism in materials dating back to the early days of quantum theory.[32] The DFT calculations that form the basis of the present work take these collective electron behavior into account. In particular in the FePt systems, the magnetic moment that forms on the Pt sites depend on their environment and the Fe concentration. This can be clearly seen in fig. 3 where the rate of change in the magnetic moment at Fe concentrations below \( \approx 15\% \) depends on the amount of Fe in the system as the induced moments on the Pt site increases, whereas above this threshold the moments on the Pt sites have reached their saturated values and the total magnetization follows the Fe and Pt concentrations.

3.1 Solid solution binary alloy dataset

In this work we focus on a solid solution binary alloy, where two constituent elements are randomly placed on an underlying crystal lattice. We use a dataset for FePt alloys available through the OLCF Constellation [22] which includes the total enthalpy, atomic charge transfer, and atomic magnetic moment. Each atomic sample has a body centered tetragonal (BCT) structure with a \( 2 \times 2 \times 4 \) supercell. The dataset was computed with LSMS-3 [9], a locally self-consistent multiple scattering (LSMS) DFT application [10, 37]. The dataset was created with fixed volume in order to isolate the effects of graph interactions and graph positions for models such as GCNN. This produces non-equilibrium alloy samples, with non-zero pressure and positive mixing enthalpy, shown as a function of composition in Figure 2.
Fig. 2. Configurational mixing enthalpy of solid solution binary alloy FePt with BCT structure as a function of Fe concentration. The color map indicates the relative frequency of data.

The input to HydraGNN for each sample includes the three components of the atom position and the proton number. The predicted values include the mixing enthalpy, a single scalar for each sample (graph), as well as the charge transfer and magnitude of the magnetic moment, both scalars per atom (node). Although the magnetic moment is a vector quantity, we treat it as a scalar because all the atomic magnetic moments in the dataset are co-linear (all magnetic moments point in the same direction).

The dataset consists of 28,033 configurations out of the $2^{32}$ available, sampled every 3 atomic percent. For this work, if the number of unique configurations for a specific composition is less than 1,000 all those configurations are included in the dataset; for all other compositions, configurations are randomly selected up to 1,000. In order to ensure each composition is adequately represented in all portions of the dataset, splitting between the training, validation, and test sets is done separately for each composition.

At the ground state, the total enthalpy $H$ of an alloy is

$$ H = \sum_{i=1}^{E} c_i H_i + \Delta H_{\text{mix}}, $$

where $E$ is the total number of elements in the system, $c_i$ is the molar fraction of each element $i$, $H_i$ is the molar enthalpy of each element $i$, and $\Delta H_{\text{mix}}$ is the mixing enthalpy. We predict the mixing enthalpy for each sample by subtracting the internal enthalpy from the DFT computed total enthalpy as a value more relevant to materials science (more directly related to the configuration). The chemical disorder makes the task of describing the material properties combinatorially complex; this represents the main difference from open source databases that have very broad elemental and structural coverage, but only include ordered compounds \cite{5, 16, 30}. 
The range of values of the mixing enthalpy expressed in Rydberg is \((0.0, 65.92)\), the range of atomic charge transfer in electron charge is \((-5.31, -0.85)\), and the range of atomic magnetic moment in magnetons is \((-0.05, 3.81)\). Since different physical quantities have different units and different orders of magnitude, the inputs and outputs for each quantity are normalized between 0 and 1 across all data.

The total magnetization of the binary alloy FePt is strongly correlated with the concentration of Fe in the alloy, as shown in Figure 3 to the left, because only the Fe atoms have a non-negligible magnetic moment. This results in a strong (albeit nonlinear) correlation between the mixing enthalpy and the total magnetization of the alloy, as shown in Figure 3 to the right.

**Fig. 3.** Scatter plot of total magnetic moment against concentration of iron (left) and scatter plot of mixing enthalpy against total magnetic moment (right).

**Fig. 4.** The linear model predictions versus the test set of FePt data for total energy (left) and mixing enthalpy (right). Each cluster of data corresponds to a Fe concentration, ranging from 6.25% to 93.75%.
4 Numerical Section

This section first presents numerical results using a linear mixing model on portions of the training dataset associated with different compositions of the binary alloys FePt, and the performance of the linear model is interpreted in terms of the physical properties of the ferromagnetic system. Additionally, a more complex surrogate model represented by an HydraGNN model is used to simultaneously produce accurate estimates of total mixing enthalpy, atomic charge transfer and atomic magnetic moment over the entire compositional range of the binary alloy. The numerical results that use HydraGNN describe the accuracy of the model as a function of the volume of data used for training.

4.1 Numerical experiments using linear mixing model

For binary alloy, there is only one term \( V^{pp}_{nm} \) (see Eq. 1) for each shell, and we consider up to 6th shell. The dataset is randomly splitted with 80% for training and 20% for testing, and the model is cross validated among different splits. The reported model performance is evaluated on the test dataset. As shown in Fig. 3, the linear model fits perfectly to the total energy, but fails to capture the non-linear behavior of the mixing enthalpy. Since the linear model is designed for the fixed concentration, we first fit the model for each individual Fe concentration (i.e., 6.25%, 12.5%, 25%, 50%, 75%, 93.75%). The observation is that as the Fe concentration increases, the goodness-of-fit deteriorates, indicating the non-linear behavior coming from the magnetism. In Fig. 4, we fit the linear model to various Fe concentrations, and each cluster of data corresponds to a Fe concentration, ranging from 6.25% to 93.75%.

4.2 Numerical experiments using HydraGNN

Training setup The architecture of the HydraGNN models has 6 PNA convolutional layers with 200 neurons per layer. A radius cutoff of 7 Å is used to build the local neighborhoods used by the graph convolutional mask. Every learning task is mapped into separate heads where each head is made up of two fully connected layers, with 50 neurons in the first layer and 25 neurons in the second. Periodic boundary conditions are implemented using the minimum image convention. The DL models were trained using the Adam method with a learning rate equal to 0.001, batch sizes of 64, and a maximum number of epochs set to 200. Early stopping is performed to interrupt the training when the validation loss function does not decrease for several consecutive epochs, as this is a symptom that shows further epochs are very unlikely to reduce the value of the loss function. We reserve 10% of the total dataset for validation, which corresponds to 2,803 atomic configurations. The remaining 90% of the total dataset, which amounts to 25,230 atomic configurations, is used to generate different training subsets. Each training subset contains a percentage of the total training dataset, ranging from 10% through 100% with increments
of 10% across successive data partitions. As discussed in Section 3.1, compositional stratified splitting was performed to ensure that all the compositions were equally represented across training, validation, and testing datasets. Equal loss function weights were used for all properties to define the global loss function for MTL. A larger partition contains the smaller ones as subsets. The training of the HydraGNN model was performed on one NVIDIA V100 GPU.

Performance of HydraGNN on different volumes of training data The validation MSE is used to describe the accuracy of the HydraGNN model as a function of the volume of training data is shown in Figure 5. The predictive performance shows that the validation MSE decreases linearly with the size of the training data for the mixing enthalpy.

![HydraGNN accuracy for mixing enthalpy](image)

**Fig. 5.** Validation MSE of MTL training performed with HydraGNN for predictions of mixing enthalpy as a function of training data volume used for training.

5 Conclusions and future developments

In this work we have provided a comparison of two different model approaches for surrogate models to fit first principles data for alloys. The goal is to provide effective models for the energy of the system that will allow the utilization in Monte-Carlo simulations of the finite temperature statistical mechanics of these systems to enable the quantitative exploration of phase transitions. The linear model has the significant advantage in significantly faster evaluation and the small number of model parameters, which reduces the training effort. While this
linear model had been successfully applied to non-magnetic multi-component alloys \cite{19} at fixed concentrations, the present work challenges the linear model. As can be seen in fig. 4, the linear model shows deviation from the correct enthalpy prediction which is dependent on the concentration. Note that this deviation is not immediately apparent in the total energy, which in the all-electron LSMS calculations is dominated by the core-electron binding energy that does not contribute to the material behavior at the energy scale of condensed matter physics.

The use of the graph convolutional neural network allows the description of the interaction for a wide range of concentrations in a single network. As can be seen in fig. 5, the model can be improved over a large range of training data set sizes with out leading to over-fitting. As the HydraGNN architecture allows us to utilize additional physical information from the LSMS calculations, such as the site magnetization, for a multi-objective optimization of the model using multi-task training, which can lead to better physical prediction of the energy of the system. \cite{23} Thus the HydraGNN model for the FePt system does not suffer the problems of the linear model. Especially it can capture the changing atomic interactions and their connection to the local Pt magnetic moments at changing atomic concentrations. This greater capability can be attributed to the inherent non-linear character of NN models that allows more complex functional relationships to be described. Yet the advantages come at the cost of greater computational cost when compared to the linear model, but the cost is still orders of magnitude lower than the fully selfconsistent DFT calculation that it models and it also benefits from the significant development effort that has been put into the efficient evaluation of neural networks on accelerator architectures.

Thus we have demonstrated the capability of GNNs to provide surrogate models for the enthalpy of mixing of substitutional alloys and the next step will be to combine the HydraGNN energy model with the Monte-Carlo simulation of the statistical mechanics of alloy ordering and incorporate it into our active learning workflow to refine the model as the simulation explores previously unseen regions of the phase space. In combination with the recent exascale HPC systems we anticipate to apply this approach to the statistical mechanics of phase transitions in multicomponent alloys of technological relevance.

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