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CUDA-METRO: Parallel Metropolis Monte Carlo for 2D Atomistic Spin Texture Simulation

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Statement of need

Atomistic spin texture simulations are crucial for understanding and predicting the behaviour of magnetic materials at the nanoscale. These simulations provide insights into fundamental phenomena like magnetic phase transition and are thus useful for exploring novel materials (Kabiraj & Mahapatra, 2023). The Metropolis (Metropolis et al., 1953) Monte Carlo (MC) method is frequently utilised for atomistic spin texture simulations as a sampling algorithm to investigate the phase space of a system and is especially effective for calculating equilibrium properties. Efficient parallelization of Metropolis MC simulation is challenging since the evolving states are typically not independent because of the Markov property. Here we focus on simulating magnetic phase transitions under the anisotropic Heisenberg Model (Heisenberg, 1928) in a very high dimensional space, which is important for emerging two-dimensional (2D) magnetism and nontrivial topological spin textures (Augustin et al., 2021). Previous attempts for parallelization are restricted to the simpler Ising Model and not applicable to 2D materials because of their finite magnetocrystalline anisotropy, complex crystal structures and long-range interactions. MC simulation of the anisotropic Heisenberg model is very complicated owing to the large number of additional Hamiltonian calculations and interconnectivity between lattice points. The calculation scales with N^2, where N represents the dimension of a square lattice. This becomes alarming when N exceeds 100, which is a realistic estimate for investigating topological spin textures (skyrmions, merons, etc). Existing open-source software for atomistic spin texture simulations such as SPIRIT (Müller et al., 2019) or VAMPIRE (Evans et al., 2014) are based on the single spin update method. While this ensures a detailed balance condition, it is very inefficient for finding the ground state for ultra large supercells.

Here we present CUDA-METRO, a graphical processing unit (GPU) based open-source code for accelerated atomistic spin dynamics simulation. This is based on our new algorithm which simultaneously updates multiple spins irrespective of their mutual correlation and harnesses the extreme SIMD (Single Instruction Multiple Device) potential of the GPU to access the ground state of ultra large supercells in a reasonable timescale. We evaluated our code by precisely simulating complex topological spin textures and temperature-dependent magnetic phase transitions for diverse 2D crystal structures with long-range magnetic interactions. We demonstrate exceptional acceleration while finding the ground state of a 750×750 supercell from an initial random spin configuration in 9 hours using an A100-SXM4 GPU.

Summary

We consider a 2D lattice system with a periodic arrangement of atoms, where each atom is represented by a 3D spin vector. This atomistic spin model is based on the spin Hamiltonian, which delineates the essential spin-dependent interactions at the atomic scale, excluding the influences of potential, kinetic energy and electron correlations. The spin Hamiltonian of the

i^{th} atom is conventionally articulated as

$$H_i = -\sum J_1 s_i \cdot s_j - \sum_j K_1^x s_i^x s_j^x - \sum_j K_1^y s_i^y s_j^y - \sum_j K_1^z s_i^z s_j^z - \sum_k J_2 s_i \cdot s_k - \sum_k K_2^x s_i^x s_k^x$$
$$- \sum_k K_2^y s_i^y s_k^y - \sum_k K_2^z s_i^z s_k^z - \sum_l J_3 s_i \cdot s_l - \sum_l K_3^x s_i^x s_l^x - \sum_l K_3^y s_i^y s_l^y - \sum_l K_3^z s_i^z s_l^z$$
$$- \sum_m J_4 s_i \cdot s_m - \sum_m K_4^x s_i^x s_m^x - \sum_m K_4^y s_i^y s_m^y - \sum_m K_4^z s_i^z s_m^z - A s_i \cdot s_i - \sum_j \lambda (s_i \cdot s_j)^2$$
$$- \sum_j D_{ij} \cdot (s_i \times s_j) - \mu B \cdot s_i$$

Where J is the isotropic exchange parameter, the Ks are the anisotropic exchange parameters, with the superscript denoting the spin direction, A is the single ion exchange parameter, λ is the biquadratic parameter, D is the Dyzaloshinskii-Moriya Interaction (DMI) parameter. μ is the dipole moment of a single atom and B is the external magnetic field. s_i, s_j are individual atomic spin vectors. $\{s_j\}$ are the first set of neighbours, $\{s_k\}$ are the second set of neighbours and so on. The subscripts below all Js and Ks denote the neighbour set, J_1 denotes the first neighbours, J_2 the second and so on. In our code, we have limited the number of neighbour sets to be 4 since it is expected for 2D materials that the interaction energy dies down beyond that. All these above parameters except B are material specific parameters that are the inputs to our MC code.

Starting from a random spin configuration, our objective is to find the orientation of spin vectors for every atom for the ground state of the lattice system for a given magnetic field and temperature. Traditionally, single spin update (SSU) scheme is employed to solve this problem, which satisfies a detailed balance condition. In the SSU method of updating the state, a single atomic spin is chosen at random and changed, while noting down the energy shift. This new state is then accepted or rejected using the Metropolis criteria as shown in Algorithm 1, where $\beta = (k_{\text{B}}T)^{-1}$, k_{B} being the Boltzmann constant and T being the temperature. It is clear that SSU becomes extremely inefficient as the dimensionality increases.

Algorithm 1 Metropolis Selection

procedure M(H_f, H_i)
  if $\Delta H < 0$ **then**
    `Return 1 (ACCEPT)`
  else if $e^{\beta \Delta H} < R$ **then** ▷ R is uniformly random
    `Return 1 (ACCEPT)`
  else
    `Return 0 (REJECT)`

where $\Delta H = H_f - H_i$ is the energy difference between the final and initial state.

In our method, as depicted in Algorithm 2, we select multiple atomic spins at the same time and change them all at once, treating them as independent events. For any individual spin, they do not feel the effects of the other changed spins. In each of these points, we use the Metropolis criteria to accept or reject the changed spin vectors. This becomes our new state. Here P denotes the number of lattice points we are evaluating at the same time for any given state, while Γ is the batch size. Tuning Γ ensures that we can fill up our VRAM with pre-generated random numbers instead of generating $4 \times P$ numbers per step. These 4 random number arrays are further divided into an array depicting the site location n, the angle coordinates for a new random spin vector θ and ϕ, and a conditional uniform random number r, which is used to evaluate the Metropolis criteria.

At present, five different lattice types (square, rectangular, centred-rectangular, hexagonal and honeycomb) are implemented in our code since most of the 2D magnetic materials fall into

Algorithm 2 Parallel Monte Carlo

procedure STEP(Run)
  Read Initial state
  Create 4 $P \times \Gamma$ length uniform random arrays
  Process the 4 uniform random number arrays
  for $i < \Gamma$ **do**
    Slice the 4 arrays into subarrays with range $[P \times i : P \times (i+1) - 1]$
    Execute P parallel BLOCKS with these subarrays
    for each BLOCK **do**
      Evaluate H before $(T0)$ and after $(T1)$ spin change ▷ Multithreading
      Wait for all BLOCKS to finish then increment i
    Update all P spins to next state
    This state is now our next state

this category (Kabiraj et al., 2022), and for neighbour mapping, we use analytical relations (Koziol, 2020).

For a lattice of size $N \times N$, 100% parallelization would correspond to selecting N^2 spins at random. Since each spin selection and its consequent Metropolis criterion is evaluated on a separate CUDA core, it becomes apparent that we would need N^2 CUDA cores to achieve this 100% parallelization. Since the proposed algorithm may not adhere to the SSU detailed balance conditions, it yields approximate results, and there is a trade-off between parallelization/acceleration and accuracy. It is found that if the parallelization is limited to 10% of the lattice size, we obtain very accurate results with significant acceleration.

Unlike the SSU scheme, we do not extract simulation data after every N^2 spin change, rather we let it run till all the CUDA cores have sychronized and arrived at the next block check, which defines our step. To directly compare, if the SSU has 1 spin changed between each step, our algorithm will have P amount of spins changed per iteration, where P is also the number of CUDA cores used or parallelization used. In the conventional SSU, data is extracted at every N^2 (a full sweep) steps, compared to which, we would take $\frac{N^2}{P}$ steps to reach the same data point.

We validate our algorithm by accurately reproducing temperature-dependent magnetic phase transitions and intricate topological spin textures already reported in the literature, either by SSU based Monte Carlo or by Landau Lifshitz Gilbert (LLG) (Gilbert, 2004) spin dynamics, for diverse crystal structures.

In their seminal work, Mermin and Wagner (Mermin & Wagner, 1966) used the isotropic Heisenberg model to analytically demonstrate that long-range order could not exist in materials with less than three dimensions. Nonetheless, in 2017 two independent research groups experimentally proved the existence of long-range ferromagnetism at low finite temperatures in two distinct 2D crystals: CrI_3 (Huang et al., 2017) and $Cr_2Ge_2Te_6$ (Gong et al., 2017). A new frontier in nanotechnology has eventually emerged, since multiple other research groups have shown that 2D magnetism can exist in various materials, even at room temperature. Finite-size effects and magneto-crystalline anisotropy, which Mermin and Wagner did not consider, are thought to be connected to the formation of 2D magnetism. To accurately simulate the magnetic states of two-dimensional materials, the Heisenberg model must be augmented with necessary anisotropic terms. Using CUDA-METRO, we first simulate the magnetic phase transition of CrI_3 from ferromagnetic to paramagnetic with increasing temperature. In Fig 1, we reproduce the magnetic phase transition from Kartsev et al. (2020), and show the effect of parallelization with respect to the reference data. As mentioned before, we can obtain very accurate results with respect to SSU methods by limiting the parallelization at 10% or below of N^2. The temperature of the ferromagnetic to paramagnetic transition point is known as critical temperature (or the Curie point) and is extracted from the peak of the susceptibility

versus temperature plot.

Next, we demonstrate the nucleation of topological spin textures which is an emergent phenomenon in condensed matter physics and is gaining importance in information technology (Bessarab et al., 2018; Luo & You, 2021). While MC simulations of medium-sized supercells (64×64) yield quite accurate results for critical temperature calculation, observing topological spin textures, one needs much larger supercells.

Results

In these examples, we always initialize the lattice with random spin configurations. First, we simulate skyrmions in $MnBr_2$ (Cui et al., 2022) as shown in Fig 2. $MnBr_2$ is a square lattice and for this simulation, we have considered up to the second nearest neighbour. This material exhibits anisotropic DMI with an antiferromagnetic ground state. An antiferromagnetic skyrmion spin texture is accurately reproduced in our simulation, which is technologically significant due to the absence of a skyrmion Hall effect in such systems. We further study the material $CrInSe_3$ (Du et al., 2022) which has a hexagonal lattice. This simulation was conducted considering only the nearest neighbours and the formation of skyrmions is shown in Fig 2. Once again our results are in agreement with the original report. All these simulations were conducted in a 200×200 $(49 \times 49 \text{nm}^2)$ supercell and took 30s to stabilize these topological spin textures at a parallelization of 20% conducted on a V100-SXM2 processor.

In Fig 3 we demonstrate the skyrmion neucleation process for the material MnSTe (Liang et al., 2020), which has a hexagonal lattice. While we first observe several skyrmions, with evolving MCS, they disappear and the whole lattice eventually becomes uniformly ferromagnetic, which happens to be the direction of the applied magnetic field. This has not been reported in the original literature (Liang et al., 2020), possibly because of the high computational time required for a traditional SSU scheme.

In the main page [https://github.com/arkavo/CUDA-METRO/blob/main/figures/Figure_5.PNG], we further show a similar life cycle evolution for a giant skyrmion of diameter 21nm hosted in the material VZr_3C_3II (Kabiraj & Mahapatra, 2023). To host such a large skyrmion, the simulation was conducted in a supercell of size 750×750 and the ground state was achieved in 9 hours using an A100-SXM4 GPU.

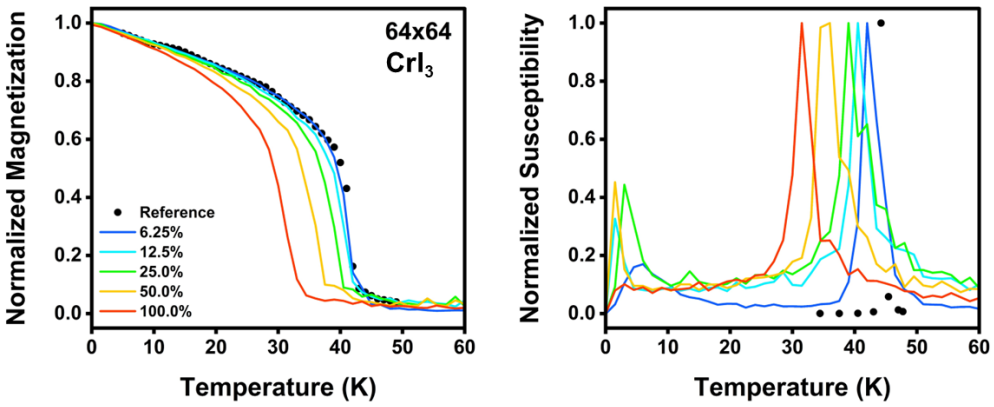

Fig 1: Discrepancy between simulation and reference (Kartsev et al., 2020) results at differing levels of parallelization. At 10%, the simulation results are almost indistinguishable from the reference data.

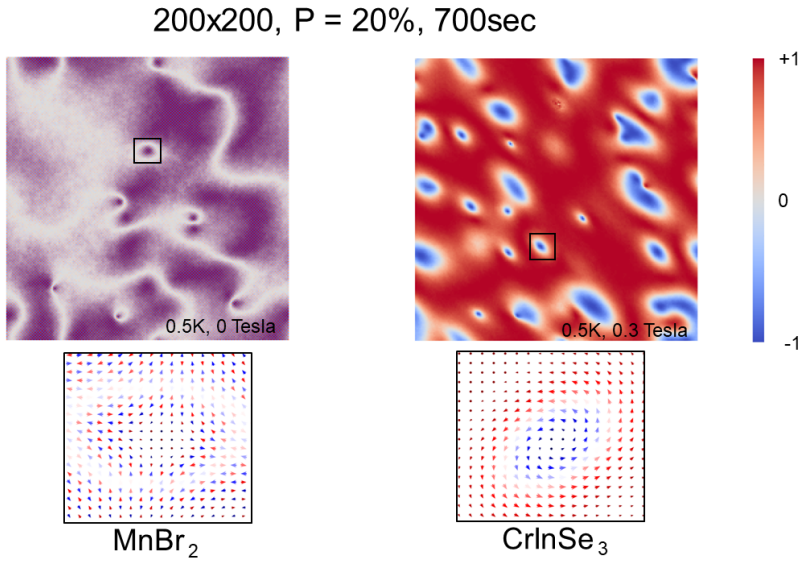

Fig 2: Presence of skyrmions in $MnBr_2$ and $CrInSe_3$. The material parameters are taken from Cui et al. (2022) and Du et al. (2022) respectively. The color bar represents normalized spin vectors in the z direction. Note that the spins of $MnBr_2$ appear purple because there are "red-blue" spin pairs for the vast majority.

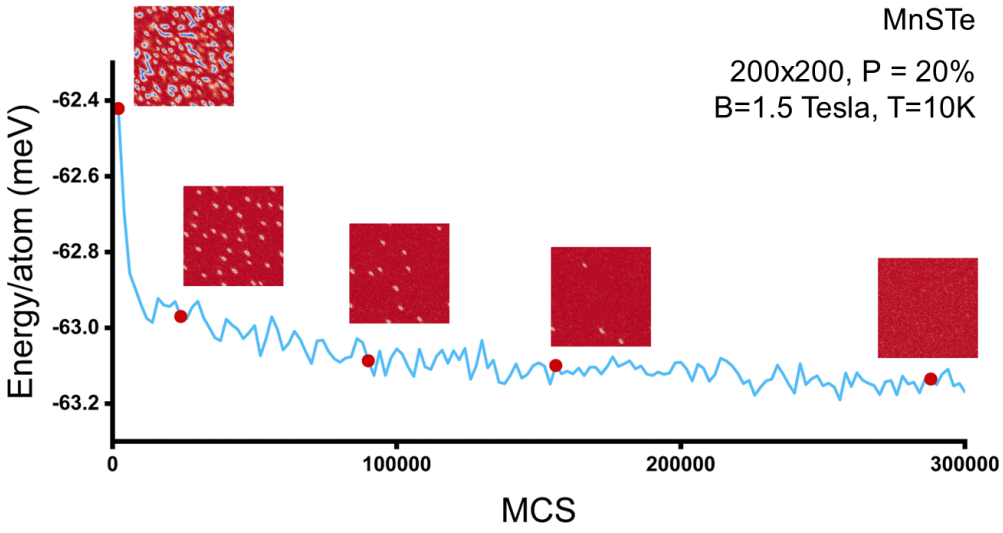

Fig 3: Lifetime of a skyrmion in MnSTe from its creation to annihilation. The graph denotes the average energy per atom. As we approach the global minima, the entire field becomes aligned to the magnetic field as expected. Total time: $30s$.

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