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# Hybrid Programming to Calculate the Susceptibility of Magnetic Materials

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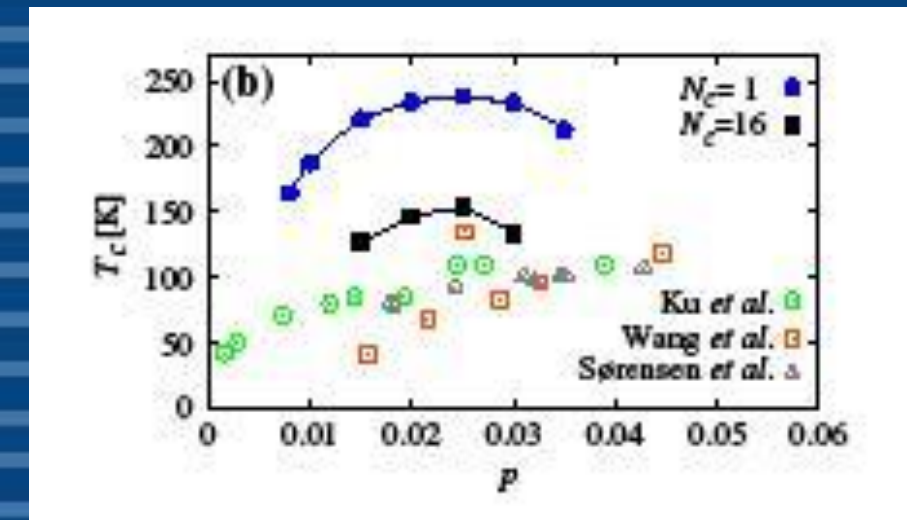
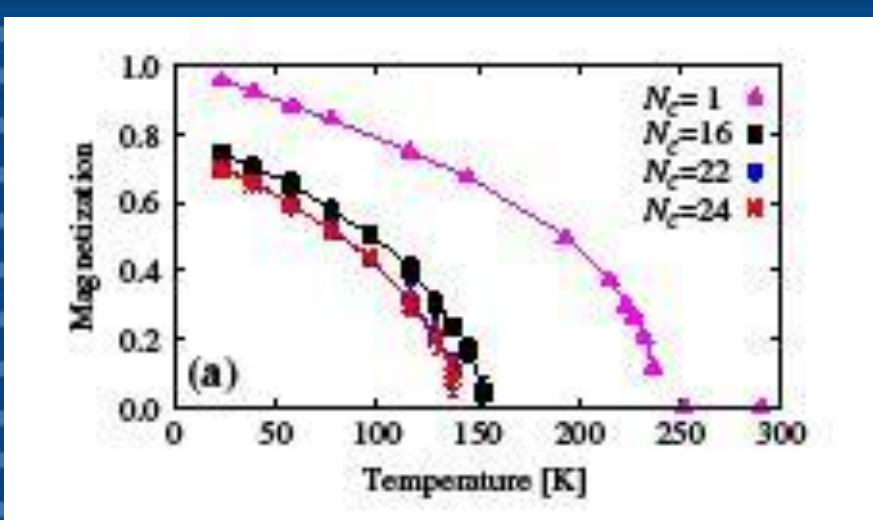


## Abstract

The purpose of this project is to be able to calculate the susceptibility of a magnetic material by more efficient means. Significant speed-up can be gained through a use of hybrid programming. By implementing OpenMP on loops in an existing MPI code, the code can be made more efficient. When the program gets a speed-up we use fewer resources such as computing power and time, thus making hybrid programming important in optimization of code. Our code also required the use of OpenMP because of the advantages OpenMP offers with the use of shared memory. Since our code deals with matrix to matrix multiplication there was not enough memory, and OpenMP allowed us to do our calculations even with our limited resources.

## Purpose & Aims

- Understand more about the properties of magnetic materials.
- We have a need for smaller more efficient devices. These materials maybe used it the next generation of devices
- Gain a significant speed-up of the program.
- Calculate the susceptibility of a two particle magnetic material.
- Learn more about the magnetic and electrical properties of a material, and allow better manipulation of these properties.

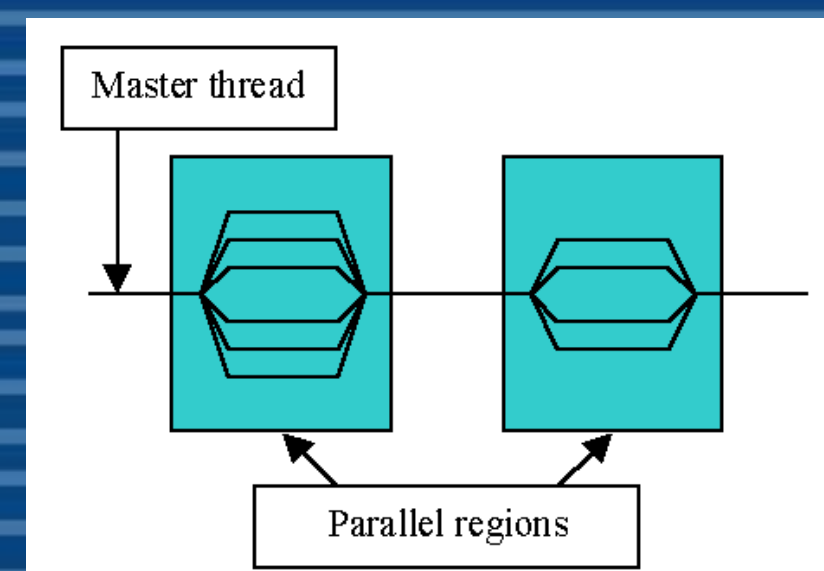


- On the left is a graph of the magnetization of Ga<sub>1-x</sub>Mn<sub>x</sub>As with Mn doping at x=.05 and the hole concentration p=.025
- The graph on the right shows the change of Ferromagnetic transition temperature as a function of the hole concentration

Yu, et al., *Phys. Rev. Lett.* (2010)

## Methods

The first week was mostly spent doing research on my topic, reading about spintronics, and learning more about the physics of the code. This required me to learn some quantum mechanics. I also needed to learn OpenMP since this would be primarily what I would be working with. I took two, week-long courses over which I learned MPI and OpenMP. I also went to the Petascale programming workshop by the VSCSE where I learned more about hybrid computing and was able to try out the new parallel computing methods I had learned. I added OpenMP to do loops that calculated matrix to matrix multiplication, and found the speed-up from the original code to the code with the added OpenMP.

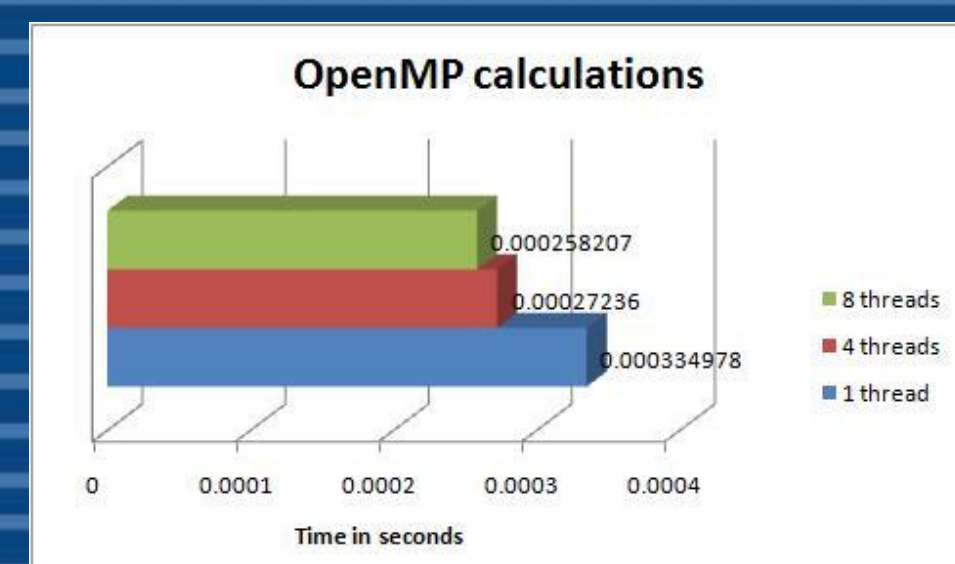


- OpenMP allows for the main program or “master thread” to create several threads within the parallel region to do the work simultaneously.

photo courtesy of  
:http://www.dartmouth.edu/~rc/classes/intro\_openmp/print\_pages.shtml

## Results

- In our initial testing code, we found that our code did not use up enough memory to see any benefits from using OpenMP.
- The testing code was too small and instead of making the code faster, actually created more overhead with each thread that was opened.
- In our other attempts we ran OpenMP and were able to see the difference in time that it took to run our code with different threads. However, there was too much memory required to run our code with MPI to get a comparison.



- The graph shows that as the number of threads increases when using OpenMP, the time it takes to complete a calculation decreases.
- We tried to compare a serial code, but there was not enough memory. The time the serial code took without any numerical computation was .00170 seconds.

## Conclusion

- Hybrid parallelization is quickly becoming a more advantageous method of parallelization
- It can allow for more improved efficiency than just OpenMP or MPI alone.
- The use of Open MP can allow computation there were not enough resources to complete previously.

## Next Steps

- Implement OpenMP to other loops
- Determine if another type of OpenMP on these loops would be more efficient
- Add OpenMP to other pragmas within the code for even greater speed-up

## References

- Yu et al. “Nonlocal Effects on Magnetism in the Diluted Magnetic Semiconductor Ga<sub>1-x</sub>Mn<sub>x</sub>As.” *Phys. Rev. Lett.* (2010)
- Wolf, S. A. et al. “Spintronics: A Spin-Based Electronics Vision for the Future.” AAAS (November 2001)
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