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Spring 2012

GPU-Based Parallel Computing for Nanotechnology Research

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Recommended Citation

McGuffey, Alex, "GPU-Based Parallel Computing for Nanotechnology Research" (2012). Celebration of Undergraduate Scholarship. Paper 156.

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GPU-Based Parallel Computing for Nanotechnology Research

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An effective technology for parallel computing is the application of graphical processing units (GPU) to computationally intensive calculations. Present research in nanotechnology simulations requires intensive calculations that have the potential to be parallelized and may benefit greatly from GPU processing. These simulations involve eigenvalue calculations on matrices with sizes up to 7776×7776 . GPU computing speeds up this core calculation by a factor of 2.5, saving hours of valuable research time. As the size of the matrix calculations increases, the speed up using GPU computing increases; however, at small matrix sizes the GPU actually takes longer to compute than the CPU.

Information about the Author:

Alex McGuffey is a senior electrical engineering student. His involvement in this research started when a fellow senior, Matthew LaRue, needed to increase the speed of his simulations for Quantum-Dot Cellular Automata (QCA) research. Some GPU computing research had already been performed and looked like a viable solution to support the QCA research. Alex will be working as a civilian in the Air Force in the Electronic Warfare Group starting in September.

Faculty Sponsor: Dr. Jeff Will

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