Abstract Submitted for the MAR07 Meeting of The American Physical Society

A uniform algebraically-based approach to computational physics and efficient programming JAMES RAYNOLDS, University at Albany, State University of New York, LENORE MULLIN, University at Albany — We present an approach to computational physics in which a common formalism is used both to express the physical problem as well as to describe the underlying details of how computation is realized on arbitrary multiprocessor/memory computer architectures. This formalism is the embodiment of a generalized algebra of multi-dimensional arrays (A Mathematics of Arrays) and an efficient computational implementation is obtained through the composition of a array indices (the psi-calculus) of algorithms defined using matrices, tensors, and arrays in general. The power of this approach arises from the fact that multiple computational steps (e.g. Fourier Transform followed by convolution, etc.) can be algebraically composed and reduced to an simplified expression (i.e. Operational Normal Form), that when directly translated into computer code, can be mathematically proven to be the most efficient implementation with the least number of temporary variables, etc. This approach will be illustrated in the context of a cache-optimized FFT that outperforms or is competitive with established library routines: ESSL, FFTW, IMSL, NAG.

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Date submitted: 15 Nov 2006

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