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Equation Solution Figures of Merit, Metaheuristic Search, and the Schrodinger Equation PAUL MACNEIL, Mercer University/School of Engineering — This presentation deals with: a definition of "equation error"; a consideration of equation solution figures of merit based on equation error, and on other measures; and the use of metaheuristic techniques in the search for approximate solutions. These considerations are illustrated by application to the Schrodinger equation for a simple system. Models suitable for computation are produced. Computation results are used to compare the consequences of selection of different figures of merit. "Equation error" is defined to be the quantity by which an approximate solution fails to satisfy an equation. "Equation error variance" is defined to be the squared modulus of the equation error summed/integrated over the domain of interest. (Generalization to sets of equations is straightforward.) In the example, equation error variance is a functional of the Schrodinger wave function. Possible figures of merit include: ground state energy, system geometry, and equation solution variance. The (derivative-free) metaheuristic used to solve the Schrodinger equation has been changed from a genetic algorithm, used in earlier versions of this research, to evolution strategy with covariance matrix adaptation.

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