

Abstract Submitted
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Where Is The Equation Solved? PAUL MACNEIL, Mercer University/School of Engineering — Considerations of solution quality for physically-significant equations often focus on observable quantities such as solution geometry, energy levels, and charge density distribution. The degree to which the equation does or does not balance, i.e., the difference between the left and right hand sides (equation error) of the equation is a mathematical measure of solution quality. The equation error will be a function of the equations independent variables, commonly including space and time. The distribution of the error, and its squared modulus, over these variables, is a quality measure for the solution. Minimization of the squared error modulus (equation error variance) integrated/summed over all allowable values of the independent variables can be used to attempt solution of the equation. These considerations are presented with examples from a simple molecular system. The distribution of equation error is visualized. Numerical experiments compare use of equation error variance with the traditional energy minimization via the variational method. The minimization of equation error variance and energy is performed by Particle Swarm Optimization (PSO). Some characteristics of equation error variance minimization become apparent from the results of these experiments.

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