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Using Genetic Algorithms to Converge on Molecules with Specific Properties STEPHEN FOSTER, NATHAN LINDZEY, JON ROGERS, CARL WEST, WALT POTTER, Dept. Math and Computer Science, Southwestern University, SEAN SMITH, STEVEN ALEXANDER, Dept. Physics, Southwestern University — Although it can be a straightforward matter to determine the properties of a molecule from its structure, the inverse problem is much more difficult. We have chosen to generate molecules by using a genetic algorithm, a computer simulation that models biological evolution and natural selection. By creating a population of randomly generated molecules, we can apply a process of selection, mutation, and recombination to ensure that the best members of the population (i.e. those molecules that possess many of the qualities we are looking for) survive, while the worst members of the population “die.” The best members are then modified by random mutation and by “mating” with other molecules to produce “offspring.” After many hundreds (or thousands) of iterations, one hopes that the population will get better and better—that is, that the properties of the individuals in the population will more and more closely match the properties we want.

Prefer Oral Session
 Prefer Poster Session

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