Exercise 4 Genetic algorithm

Read the following general description of a genetic algorithm:

> In a genetic algorithm, a population of candidate solutions (called individuals, creatures, or phenotypes) to an optimization problem is evolved toward better solutions. Each candidate solution has a set of properties (its chromosomes or genotype) which can be mutated and altered.
>
> The evolution usually starts from a population of randomly generated individuals, and is an iterative process, with the population in each iteration called a generation. In each generation, the fitness of every individual in the population is evaluated; the fitness is usually the value of the objective function in the optimization problem being solved. The more fit individuals are stochastically selected from the current population, and each individual's genome is modified (recombined and possibly randomly mutated) to form a new generation. The new generation of candidate solutions is then used in the next iteration of the algorithm. Commonly, the algorithm terminates when either a maximum number of generations has been produced, or a satisfactory fitness level has been reached for the population.
>
> A typical genetic algorithm requires:
>
> - a genetic representation of the solution domain,
> - a fitness function to evaluate the solution domain.

a) What type of optimization routine is a genetic algorithm?

b) If one would like to use it for a geometry optimization of a molecule what would be a good representation of the system?

c) And the fitness function?

d) How would you make a starting population?

e) Could you think of a good mutation and recombination scheme?

f) What would be the role of both functions?

g) Repeat questions d and e for a crystal (of known and unknown structure).

Exercise 5 Verlet integrator

Show that the Verlet integrator is time reversible. Why is this important (two reasons)?

Do the same for the Leap Frog integrator.