Using Darwin to discover new advanced materials

The process of evolution, first described in detail by Charles Darwin, has resulted in the amazing diversity of plants and animals in our world, each subgroup shaped by the effects of the different environments in which they live. Each population of individual in a given environment are slightly different, and those with a more favorable set of skills or adaptations will tend to survive better and reproduce more successfully – essentially the 'survival of the fittest'. Surprisingly, scientists have now learnt how to mimic this process and use it to design new drugs, catalysts (materials that greatly speed up chemical reactions), and other advanced materials that are making a big impact on the technologies upon which we all rely.

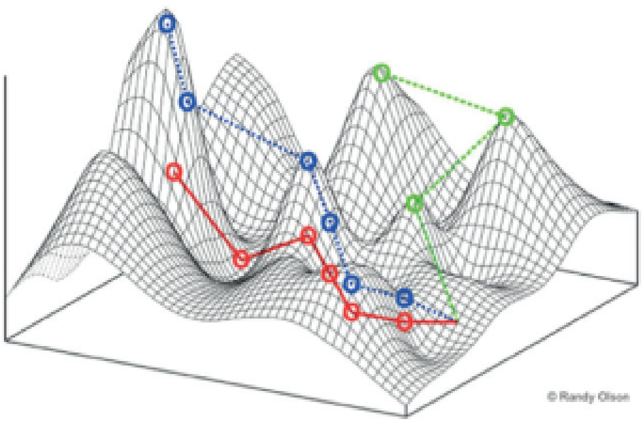

Diagram of an 'evolutionary landscape' that shows how genetic algorithms can find the tops of the peaks that represent locally optimal properties (no mathematical method can local the best peak on a complex landscape except by exploring every part of it)

A molecule or other material like a polymer (plastic) can be described by a series of numbers that capture what kind of atoms the material is made from and how the atoms are joined together (which is called the materials 'genome' by analogy with the information containing genes in living things). Other research that we and others have done has shown that these numbers are related in a complicated way to how the material performs e.g. Its strength, ability to treat a disease, suitability for making LED TV screens etc. This desired performance is called the materials 'fitness'. To 'evolve' a material, we make a small number of materials (called the initial 'population'), generate the numbers that describe the structures and other molecular properties of them, measure the property that we are interested in improving (the 'fitness'), and selecting those members of the population that are the best performing. We then alter the numbers (genome) that describe the material, equivalent to causing a mutation, or we mix the 'genomes' of some of the best materials together (equivalent to breeding in living things) and generate a new population of materials that are fitter than the old set. We again measure how well these perform, mutate those that are best, generate another population, and continue this cycle until we get some materials that

are good enough for our purpose. As the number of possible materials that could be made is essentially infinite, these evolutionary methods are very effective for quickly finding useful materials from a very large number of possibilities, in a relatively small number of experiments. Coupled with the increasing use of robotic systems to generate large number of materials (e.g. The CSIRO RAMP facility in Melbourne
Australia http://www.csiro.au/en/Research/MF/Areas/Chemicals-and-fibres/RAMP), they will undoubtedly play an important role in the development of amazing new materials for healthcare, regenerative medicine, energy and other uses in the near future.

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