non-homologous three-helix packings observed, seven are described by the first model and one by the second[1].

The quasi-spherical polyhedron model for the packing of helices has important implications for fields outside protein folding. Similarities in the structures of proteins are often taken to imply evolutionary relations even if there is no significant homology in sequence. Such a relation may exist. But Murzin and Finkelstein show that helical proteins can have very similar architectures independent of both sequence homology and chain pathway. Helix packings from non-homologous proteins but whose geometry is described by the same model appear very similar. Indeed, helix packings whose connectivities are very different but which fit the same model have sets of alpha carbon atoms that superpose with a root-mean-square difference in position of less than 2.5 Å. Values somewhat greater than this have previously been taken as clear evidence for evolutionary relationships. □

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Computation

Breaking the matrix speed limit

Steve McCormick

MATRICES abound in the sciences. Many problems involving inter-related variables can be cast into equations that use the familiar array form of a matrix. For large-scale problems involving many variables, the matrix in question is often composed mostly of zeros — a so-called sparse matrix. To capitalize on this structure, the equations can usually be solved by iteration on a computer. Unfortunately, the asymptotic approach of the iteration to the solution can become extremely slow, a process termed critical slowing down. Among the many possibilities for combating this stumbling block, that now used by R. G. Edwards *et al.* (*Phys. Rev. Lett.* **61**, 1333–1335; 1988) in a model problem shows great promise.

Sparse matrices arise in the modelling of large, complex phenomena from virtually every corner of science, including fluid mechanics, structural analysis, molecular dynamics, geodesy, economics, image reconstruction and X-ray crystallography. A sparse matrix expresses known local rules that govern the behaviour of a system of objects describing the phenomenon of interest. These rules characterize direct interactions that emerge as numbers in the matrix array. The numbers in a given row quantify the interaction of a given object with all of its neighbours. The location of the relatively few non-zero numbers in the row indicate who the neighbours are, and their magnitudes indicate the degree of the interaction. The actual behaviour of the system can be recovered numerically by solving a set of equations defined by the matrix, but conventional methods for solving these equations often suffer from the debility of critical slowing down.

In their new work, Edwards *et al.* investigate this sort of trouble in the context of certain lattice systems that arise in the study of random-resistor networks, quantum chromodynamics and discrete Schrödinger operators. (For example, random-resistor networks are a paradigm for the conduction of current through composite materials. The non-zero matrix elements correspond to resistors randomly placed between neighbouring points of a lattice, and the idea is to determine the current at these points for a given external current supplied to the lattice.) The cure Edwards *et al.* use involves a relatively new method, called algebraic multigrid (AMG), the basic idea of which can be described as follows.

Conventional methods start with a given approximation to the state of the system, then attempt to make improvements by a sequence of sweeps that adjust the state of each object in the system, forcing the objects in their turn to obey the local rules. Critical slowing down occurs after a few such sweeps because these local adjustments can take an inordinate amount of time to determine the global state of the system. This is not unlike the trouble that an ant has in building or, better, rebuilding an ant hill. AMG avoids this trouble by making additional improvements on more global scales.

This is accomplished systematically by aggregating the objects into groups, automatically translating the local rules to apply to the aggregated system, then sweeping through these groups to make adjustments at the aggregated level. This approach gives an ant the power to work with clusters of sand for adjusting the coarse features of the hill, reserving the delicate manipulation of individual grains for the finer features. It gives the researcher the ability to determine the state of a system at a cost equivalent to just a couple of sweeps of the conventional method.

This approach is often relatively easy to develop, at least in principle. For lattice systems, there is usually one property (or variable) used to express the local rules among the objects, and this property can be treated as sort of a metric to determine appropriately how the objects and local rules should be aggregated. For example, in random-resistor networks, the resistance between two sites that are geometric neighbours can be interpreted as a measure of the intervening distance. Sites that are close in this sense can be grouped, and the aggregated rules can be determined by an averaging of the individual rules based on this measure. AMG computer software that automatically implements this approach has indeed been fairly successful for lattice systems, elliptic fluid flows and various other applications.

But for other complicated phenomena, development of the AMG approach can require very substantial research. For example, many systems use two or more properties per object to define local rules. In structural analysis, displacements for each coordinate and rotations for each pair of coordinates determine the state of the system. In developing an AMG scheme for a new problem of this type, just how such properties should be used to form distance measures is not always clear at the outset. But there have been very successful designs of AMG techniques for a broadening class of applications, including least-squares problems in geodesy, general fluid flows and various structural-analysis problems (see *SIAM Frontiers in Applied Mathematics* Vol. 3, ed. McCormick, S. F.; SIAM, Pennsylvania, 1987).

But this is just the beginning. Led by its pioneer A. Brandt and others, the multigrid concept has been making dramatic inroads into many new areas of science (see *Lecture Notes in Pure and Applied Mathematics* Vol. 110, ed. McCormick, S. F.; Springer, New York, 1988). Several challenging problems that were previously thought to be intractable now seem ready to fall before the multigrid axe. In the field of quantum chromodynamics, it is estimated that conventional methods could take ten million years or more to determine the mass of a proton. A novel multigrid approach seems to hold the promise of reducing this time to perhaps as little as a few hours. If such dramatic improvements can be made in this and other challenging fields, then critical slowing down may be well on its way out of scientific computation. □

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