Reticular or Articulatory Geometry

[net]

Artifacts found at Blombos, about 75,000 years old, including red ochre stone with design carved in it; see Blombos Cave Project.

Humans have long found the business of successfully articulating precise things together rewarding, both economically and psychologically. In addition, precise articulation is necessary in order to make things come out right, from the construction of temple complexes to carving stone balls with curious symmetries. The necessity and inspiration of articulation in geometric figures suggests that this ancient field of geometry really should be called "articulatory geometry" -- and indeed, it is not difficult to find the adjective "articulatory" and the noun "geometry" in close proximity in mechanical engineering and anatomy papers.

"Articulatory" has a more distinguished pedigree than "reticular". Unlike the latin **rete**, which simply appeared in ancient Rome from who-knows-where, the coincidence of the latin **artus** (joint) and **articulus** (joint, precise point, or division), related to **armus** (arm) and hence to **ars** (art), seems connected to the Hittite **ara** (something that fits) and the Sanskrit **irmas** (arm): the word seems to trace to Indo-European roots, suggesting that the art of fitting things together (as one might punningly describe architecture) has been a longstanding focus of attention in Eurasian civilization.

The word **reticular** *is derived from* **rete**, *a latin word "of obscure origin" that means* **net**. *In English, an object is "reticular" if it is intricate and netlike, consisting of many articulated components.*

The word **geometry** *is a Greek concoction, meaning "the measurement of the Earth"; this etymology refers to the traditional view (advanced by Herodotus) that geometry was invented by Egyptian (and perhaps Mesopotamian) surveyors. However, there is archeological evidence of interest in polyhedra and other geometric objects (e.g., right; in fact, all five Platonic solids are represented -- in a sense -- among these ancient Scottish balls).*

Omar Yaghi has denoted as **reticular chemistry** *that part of nanoscience and materials science concerned with the assembly of large or potentially unbounded structures composed of many articulating parts. Similarly, Georg Alexander Pick's theorem on the areas of polygons formed by families of parallel lines on the plane inspired fans to dub his work on the geometry of such net-like objects* **reticular geometry**, *(although the phrase is obscure enough that as of September, 2010, the AMS MathSciNet had never heard of it.) And so we dub as* **RETICULAR GEOMETRY** *that area of geometry concerned with large and complex geometric objects consisting of many articulating components.*

Of course, the use of the adjective "reticular" instead of the adjective "articulatory" suggests a bias in favor of studying the final, fully assembled geometric structures, rather than the details involved in the design process. This is a bias that geometers should avoid in practice, although it is quite possible that the mathematics of the two different aspects of this geometry are different (and in fact, there is anecdotal evidence that the mathematics of the final structures in reticular geometry is more difficult than the mathematics of the assembly process in articulatory geometry).

On this page:

- Reticular Geometry and Design. Much of the interest in what we might call "reticular geometry" has been driven by economic demand, by the need to design complicated objects.
- Reticular Geometry as Mathematics. Nevertheless, the problem how how to fit together many geometric objects is ultimately a mathematical one, associated with several extant fields of mathematics.
- The Sociology of Reticular Geometry. On the other hand, there is a long history of popular interest in the sorts of shapes people try to fit together, and how to fit them together.
- My Adventures in Reticular Geometry. I'm currently working on courses in the subject while doing some research, in particular on Euclidean graphs as models of crystal structure.

Image of carved stone balls, approximately four millennia old, from Scotland's University of Glasgow's Hunterian Museum; image from Wikimedia Commons.

Figurines and other decorative pottery go back several tens of thousands of years, but we do not know when humans first started *creating* art, as opposed to collecting things in Bower-bird fashion. Of course, it is likely that most of our ancestors collected artificial things made by artisans just as we collect bric-a-brac made by local artists or manufactured by big companies. One of the great holes in our history and archeology is what people did collect or create: just as nowadays, people collect ugly clocks, Elvis statues, and crystal pyramids, it seems likely that ancient people collected *something*. If so, collectibles were probably collectible because of their novelty -- like fossils and crystals.

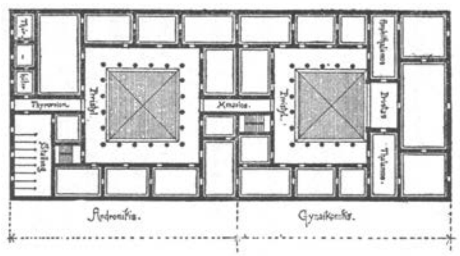
Objects associated with reticular geometry have always been popular, and have always exerted influence on our esthetics. Once artificial objects appeared, what were they? And were they designed in advance or did artisans just feel their way?

Reticular Geometry and Design

Between thirty and forty thousand years ago, people started making vast numbers of things, and the repertoire of human technology expanded dramatically. No one knows the reason for this "Paleolithic

Reticular Geometry as Mathematics

William C. Waterhouse (of Pennsylvannia State University) suggested in a paper, Discovery of the Regular Solids, that polyhedra were inspired by the discovery of crystals. There is little direct evidence of this, but revolution", although explanations range from new trade routes to mutations. Whatever the reason, the result was that people now had a need (or a desire) for designing all sorts of new blades, baskets, boats, and whatever else the growing tribes demanded. We don't know much about their design processes, but by later Antiquity, during the Roman era, there was a formal design process by which people designed buildings, bridges, and other large structures.



Greek house plan after Vitruvius, posted in Wikipedia Commons.

Reconstruction of the palace at Knossos, posted in Wikimedia Commons.

Marcus Vitruvius Pollio's Architecture, written in the first century B.C., is the oldest architectural text known, and is an example of the interplay between geometry and engineering. More precisely, between *reticular* geometry -- in that architecture relies on the articulation of many parts -- and the design of complex structures.

Vitruvius' *Architecture* is an example of applied reticular geometry: it was an account of the structural elements, the properties of the materials used to realize those structural elements, together with some guidance on how to assemble the desired building.

But clearly, Vitruvius' text was describing well-understood contemporary information in architecture and engineering, as can be seen from much older and yet very sophisticated structures around the Mediterranean. For example, the Minoan palace of Knossos in Crete, which was constructed and reconstructed repeatedly during the second millennium B.C., clearly was the result of repeated and incremental but still intelligent design: it had stone stairs supported by wood pillars (which meant that it required careful planning), a working sewer system, and careful placement and sizing of windows to light interiors. Although no accounts of the design of the palace survive, it was clearly designed by engineers who were geometrically sophisticated.

In fact, not only the standard geometry of surveying, but the reticular geometry of fitting things together, are apparent in ancient structures like the Anasazi complex now known as Pueblo Bonito, even though the societies that built these structures appear to have been at best semi-literate, and left no texts for historians to attempt to translate. That should not be surprising, for agriculture entails the geometry of surveying, and once one starts to build things, one has to fit things together. Reticular geometry may be one of the first fruits of any agricultural revolution.

Moving forward, during the "High Middle Ages" (roughly the 11th, 12th, and 13th centuries), Europeans making the pilgrimage to Santiago de Compostela visited the embattled provinces of Andalusia -- roughly that part of the Spanish peninsula under Islam -- and marveled at the architecture. The inspiration followed them home, where they built Gothic cathedrals, which were not quite as organized as their Andalusian models (like the Alhambra), and which occasionally fell down during construction. But stonemasons gradually figured out how to wing it, and during the remainder of the Middle Ages, they filled northern Europe with cathedrals of light. But the Mediterranean had much better light than northern Europe, and as the Middle Ages waned into the Renaissance, the Mediterranean also had more money.

very little is known about scholarly, professional, or folk interest in polygons, polyhedra, tilings, or similar structures before Kepler; we have a few scattered literary works and a lot of art, architecture, and engineering. And even today, interest is scattered about in a variety of fields, and while many of us are familiar with the usual suspects -- the Platonic solids, the Archimedean Solids, and the Catalan Solids, much of the research in polyhedra is concerned with something other than polyhedra in mind. And as for putting things *together* like so many legos...

Self-portrait (drawing) of Albrecht Durer, posted on Wikipedia Commons.

[Kepler]

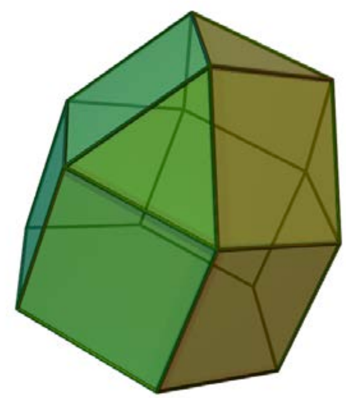
Portrait of Johannes Kepler, posted on Wikipedia Commons.

Polygons, polyhedra, and other shapes permeate the artistic and engineering worlds of many cultures, but the mathematical attention is less clear: it appears spotty, but the record is fragmentary, so we actually don't much about this kind of geometry prior to the Renaissance, when Europeans got interested in them. Albrecht Durer wrote much about his interests, and was a draftsman whose work helped inspire descriptive geometry; his *Painter's Manual* introduced the notion of a *net* of a polyhedron, which was essentially the graph of its vertices and edges. Johannes Kepler subsequently conducted a more mathematical investigation, particularly of atomic arrangements of matter (in *A New Year's Gift of Hexagonal Snow*) and of the relationship between polyhedra and astrology -- er, astronomy -- in *Harmonies of the World*.

It is true that polyhedra -- or rather, their umpteen-dimensional analogues, polytopes -- are very big business nowadays. Literally. One of the primary objects in Combinatorial Optimization is the solution space to a system of simultaneous linear equations, which is the object of linear programming. If we represented each linear equation as a half-space in some dimension, the solution space to the entire system would be a convex polytope, and since businesses and governments use linear programming to make optimal allocations of scarce resources, umpteen dimensional polytopes have been all the rage ever since the British government used it to keep afloat during World War II.

But we are interested in how (geometric) things can be taken apart and put back together. Algebraic topology is interested in the related problem of taking apart and gluing together topological objects -- objects that can be continuously distorted -- and we can borrow some of the topological machinery. Machinery that probably traces its provenance back to Durer's nets, anyway.

One of the basic and most familiar dissections of a polytope is into cells that make up its interior and boundary. For example, the complex (e.g., CW-complex) of a polyhedron is the partially ordered set (poset) consisting of its vertices, its edges, its faces, and its interior, ordered by inclusion. Such a dissection into *cells* can be conducted on polytopes of arbitrary dimension. But for our purposes, we may be even more interested in the proposal that we can have arbitrary complexes, i.e., any poset of cells ordered by inclusion such that every boundary cell of a cell in the complex is also a cell in the complex. These complexes are indeed complicated arrays of geometric objects that are organized in space to fit together, and thus would appear to be typical objects of reticular geometry.



A "Johnson solid", an elongated triangular cupola, posted in Wikipedia Commons. The complex consists of the central three-dimensional interior, the fourteen faces (two-dimensional cells), the 27 edges (one-dimensional cells), and the 15 vertices (zero-dimensional cells).

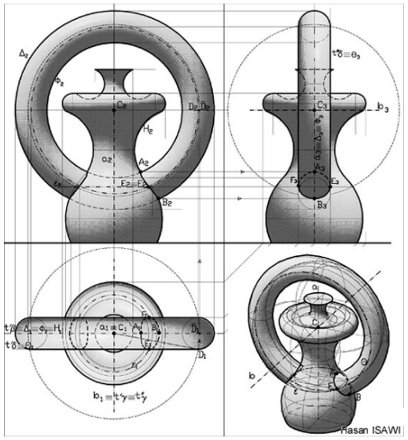
The cathedral of Santa Maria del Fiore, completed by Brunelleschi, posted in Wikipedia Commons.

One of the challenges symbolic of the Renaissance was the decision of the City of Florence to build a dome on top of the Florence Cathedral of Saint Mary, even though no one had built a dome that large since the Pantheon over a millennium earlier. (Even worse, no one knew how the Pantheon had been built, or even what, exactly, the Pantheon was made of -- it turned out to be reinforced concrete.) Worse, the one thing that they did know was that building the scaffolding for the dome of the Florence cathedral was impossible. To top it all off, some silly people wanted a lantern (a structure like in the one on top of the dome at right) on top, even though the Pantheon at least did not have that complication.

Filippo Brunelleschi's solution -- which involved careful (if secret) designs, developing a construction process in which the partially built dome and the scaffolding supported each other, on top of the Middle Eastern device of having a heavy but hidden dome between two light but pretty shell domes -- was a dramatic example of the ability to build intricate structures designed in advance.

It is not coincidental that Brunelleschi was one of the pioneers of perspective drawing and painting, for the problem of what a structure is and what it looks like was at the center of art and of architecture in the Renaissance, for artists were working away from the abstract and symbolic art of the Middle Ages, while architects were discovering that when they wanted to design genuinely novel buildings, it was a wise idea to have a clear design in mind *before* they started building.

Albrecht Durer carried perspective into *description* (of military fortifications) and so *descriptive geometry* and *projective geometry* began, officially with Johannes Kepler and Gerard Desargues and continuing up to Gaspard Monge at the end of the 18th century, applying his work to military fortifications.



Images of an object from different positions, posted in Wikipedia Commons by Hasan Isawi.

Very loosely, projective geometry (in at least its original incarnation) was concerned with what an object looked like at a particular distance, while descriptive geometry was concerned with how it looked through a zoom lens -- in particular, at an infinite distance through an infinitely powerful zoom lens (notice the picture at left, considered ideally, is not from a particular distance but consists of projections onto planes, as if through an infinitely powerful zoom lens from an infinite distance). Descriptive geometry provided a tool for designing novel objects that some machinist would then try to make, and it provided a critical intellectual toolbox for the Industrial Revolution of the 19th century -- and it continues to earn a living in technical and engineering drawing.

It is no coincidence that the Nineteenth century saw the development of mass assembly, of industrial power, and of astronomer John Herschel's invention of the *blueprint*. The intuition had become, if you can draw it, you can make it. A sideways glance at Frank Lloyd Wright's fantasies suggest that that is not necessarily true: building materials matter, and there is always the detail of the assembly process itself...

During the Nineteenth century, a new kind of structure appeared. As scientists began to consider the possibility that matter was composed of tiny and somewhat-divisible particles called *molecules*, themselves composed of even tinier and possibly indivisible particles called *atoms*, people began to wonder what these molecules might look like.

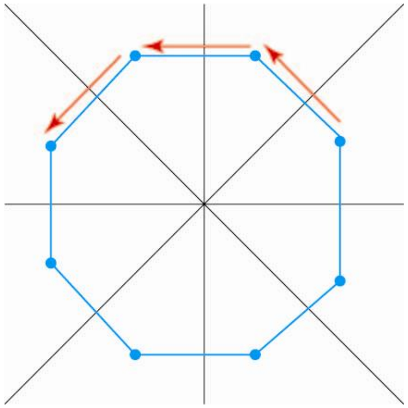
But how to put such complicated complexes together? In order to do this, we probably have to shock the purists by taking pliers and crowbars to the standard definitions, but it's a free country and geometers are already taking liberties, so...

While H. S. M. "Donald" Coxeter's primary concern seems to be more the shapes of individual things than putting many things together to make complicated things, he did dissect many polytopes into individual pieces and in the process helped develop much of the machinery available to the contemporary reticular geometer. From the point of view of most contemporary geometers and algebraists, what Coxeter created was a very useful system for representating algebraic objects.

- Coxeter's dissection techniques, applied to very nice (highly symmetric)complexes, would produce a *chamber system* of cells laid out in space, complete with an adjacency relation.
- Meanwhile, mathematicians developed Group Representation Theory, whose ultimate program is to take a horribly complicated and therefore unintelligible group, and find an isomorphic group that was a nice group of permutations of some nice set -- often, a nice group of linear transformations on a very nice (perhaps even real or complex) vector space.
- One collection results are the Coxeter Groups, the peanut butter cup of chamber systems embedded in spaces such that for such a chamber system, there is a nice group of transformations which, when applied to the space the chamber system is embedded in, permute orbits of chambers around.

There are all kinds of restrictions, generalizations, and other variations of the above, including buildings (for which Jacques Tits won the Abel Prize, the highest prize in mathematics). In all this, we can see that geometry is now in service to algebra, as can be seen by the very title of, say, Michael Davis's book on The Geometry and Topology of Coxeter Groups. Whether Coxeter would approve of Geometry being the handmaiden of algebra is another matter.

But of course, geometers could turn the relationship around...



Imagine the plane chopped into eight pieces by four mirrors, from which we get four reflections. Those four reflections generate a dihedral group (of order eight) of isometries of the plane. We could regard those eight pieces as eight vertices, with an edge relation representing adjacency, giving us a cyclic graph. Then the four reflections generate a dihedral group (of order eight) of automorphisms of that graph. With only one orbit of vertex, this Euclidean graph represents a uninodal or vertex transitive net, with which Richard James can model "objective structures". Image on this website, released to the public domain.

Let me give an example. A reflection in Euclidean space is an affine transformation that *reflects* points across some line (in two-dimensional space), plane (in three-dimensional space), or other hyperplane in Euclidean space. And a Reflection Group is a group generated by reflections.

In a Wythoff Construction, one starts with a fundamental region of a reflection group (i.e., a closed polyhedron that intersects each orbit of the reflection group at least once while its interior intersects each orbit at most once). Then one applies the elements of the reflection group to the fundamental region to get copies of it (which are also fundamental regions), and these copies cover the entire space, although the intersection of any two copies of this fundamental region intersect (if at all) only within their boundaries. The result is a tessellation of the original space, and this tessellation tells the algebraist something about what the reflection group looks like.

But one can use the same approach to build, say, a Euclidean graph whose vertices represent, say, atoms, and whose edges represent, say, chemical bonds. Embedding a fragment of a graph inside a putative fundamental region, one obtains a Euclidean graph that might be an interesting object in itself -- perhaps, as hoped by the

Models of molecules -- including August Wilhelm von Hoffman's stick-and-ball models -- appeared in the later Nineteenth century, even before there was a consensus in the scientific community about atoms and molecules. They were, as George Polya pointed out, combinatorial objects, and thus graph theory could be used to model molecules. But they were also geometric objects.

Isomers are molecules with the same chemical formula -- the same number of each kind of constituent atom -- and yet are structurally different. One notorious kind of (pair of) isomers are the stereoisomers, i.e., two molecules that are mirror images of each other. This issue of chirality -- of mirror images, of right- and left-handedness -- became one of the central issues in *stereochemistry*, although it involves the spacial relationships between atoms in a molecule, or between molecular building blocks (MBBs) in a super-molecule.

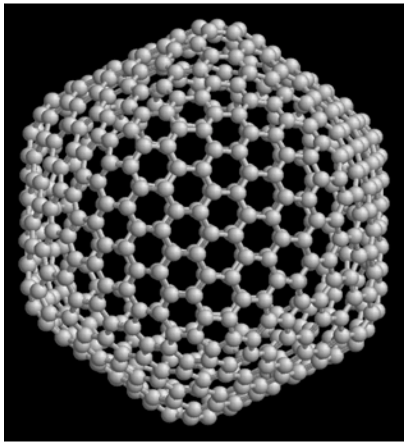


Image of Fullerene c540, an example of a fullerene, i.e., a finite carbon structure in a graphene-like (graphite-like) arrangment. Fullerenes were named after architect and geometric enthusiast Richard Buckminster Fuller. Image posted in Wikipedia Commons.

During the early Twentieth century, new techniques for determining the structure of molecules pushed geometry into the foreground. But during the later Twentieth century, something new arose: the ability to control molecular building blocks, or even individual atoms, allowing chemists to design and assemble novel structures. As Richard Feynman predicted in an influential address on There's Plenty of Room at the Bottom, this led to a qualitative change in science and engineering. During the last few decades, scientists have assembled graphite-like polyhedra, DNA complexes, artificial proteins, and other nano-objects. As the target products get more complicated, the mathematics of the design principles get more sophisticated, and a demand appears for more effective mathematics for more effective design.

The notion that all matter is composed of tiny particles is ancient: the Greek philosophers Democritus and Epicurus championed the notion, which Aristotle refuted (at least to the satisfaction of the Europeans). The atomic theory was resurrected by Johannes Kepler and Robert Boyle, and very quickly became central to crystallography, for crystallographers from Nicolas Steno to Rene Hauy found that they could explain the polyhedral shapes of crystals by assuming that crystals were composed of very regular arrays of tiny something-or-others. The Nineteenth century saw the protracted foodfight over the atomic theory, and crystallography was at the center. The structure of crystals made sense if they were composed of something like atoms or molecules. And although the final argument for the atomic theory was based on molecular motion -- the only viable explanation for Brownian motion (the habit of dust particles floating on water to jiggle about randomly) seems to be Albert Einstein's proposal that tiny particles are jostled by even tinier molecules -- the success of the atomic theory in crystallography helped set the stage.

creators of the Symmetry-Constrained Intersite Bonding Search (SCIBS), a geometric representation of the atomic structure of a zeolite crystal.

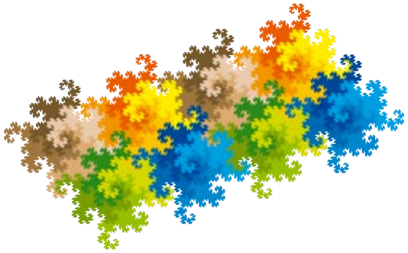
Traversing graphs -- Euclidean or otherwise -- using transformations that are (when restricted to those graphs) automorphisms brings us to the group theory that consists of:

- Taking a group and labelling a set of generators with symbols, and then
- Assigning to each element of that group a list of those symbols -- a word -- encoding a composition of generators that will produce that element.

This leads us to Geometric Group Theory. One thread through the work of Jean-Pierre Serre and the work described in Warren Dicks & Martin Dunwoody's book on Groups acting on graphs is the use of words to encode traversals of graphs. And if the group one starts with is particularly nice, its word problem may actually be solvable by a automaton, making it an automatic group; the crystallographic groups are automatic, and these are many of our most important examples at the moment.

Wythoff constructions are only one source of tessellations, and tessellations form a broader class than just (near) partitions into fundamental regions. Typically, a tiling (tessellation) is a covering of a Euclidean space by finite (bounded) closed sets (called *tiles*) such that:

- Any two tiles are either disjoint or intersect across their boundary, and
- There are finitely many congruence classes of tile.



Tiling by "dragon curves", posted in Wikipedia Commons.

Two of SCIBS's competitors work by enumerating tilings (or more precisely, Delaney-Dress symbols representing tilings), and then:

- In the case of the algorithm developed by John Huson, Olaf Delgado-Friedrichs, et al, interpreting the tiling of 3-space as crystal, or
- In the case of the Euclidean Patterns in Non-Euclidean Tilings [EPINET] program, taking a tiling of a 2-dimensional hyperbolic space and wrapping it around a nice and known 3-dimensional structure to get a novel structure.

The most standard classification of tessellations are into the *periodic* and aperiodic; a tessellation is *periodic* if there is a basis of its underlying vector space such that any translation of the tessellation maps the tessellation onto itself: it repeats in axial directions. Periodic tessellations are often treated as models of crystal structure, while aperiodic tessellations have been used (depending on regularity properties) to model a range of materials from quasicrystals to glasses.

A related structure is the packing, in which structures are embedded in space like a tessellation, only they no longer have to cover the space they are embedded in. The standard issue is usually making all the objects fit.

Taking a larger perspective beyond assembling solid rigid objects in a vacuum to be connected at particular junctions, there are several directions in which we can generalize:

- *Are these objects rigid?* If we permit them to be completely "flexible", we are in a situation more readily dealt with using topology. However, there may be intermediate situations in which one is dealing with components that are somewhat rigid. While the mathematical theories of rigidity tend to be aimed at a more binary situation -- objects are rigid or they are not -- recalling the practical example of basket-weaving, the problem of partial rigidity seems a serious one.
- *Are the junctions rigid?* This brings us to the classical theory of geometric rigidity, which certainly goes back to Antiquity (architects have long known about bracing frameworks), and has become a field of mathematics during the last two centuries.
- *Do we require contact at junctions, or do objects "fit" in accordance with some kind of action (or junction) at a distance?* For example, an ionic crystal (like salt) consists of many positively and

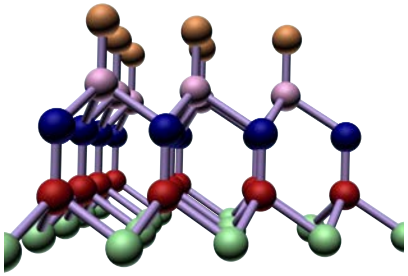


Image of cubic diamond lattice, posted in Wikipedia Commons by Rosario van Tulpe.

But that means that materials are themselves extended geometric structures, perhaps best envisioned as infinite structures filling space. If the structure was a regular array at a nanoscopic level, one could imagine that the resulting crystal would tend to have cleavage planes and various rotational and mirror symmetries. From cleavage planes, mathematicians like Augustin Cauchy devised polyhedra (just as Archimedes devised polyhedra from cleavage planes -- although there is no surviving evidence that Archimedes was inspired by crystals) (although, for all we know, he might have been). From the symmetries, physicists like Auguste Bravais and mathematicians like Yevgraf Fyodorov devised the crystallographic groups in a massive effort that spanned the Nineteenth century and the careers of many scientists.

In the early Twentieth century, physicists and chemists devised methods for determining the structure of materials. Since then, chemists have developed methods for designing crystals *and then* building them, as opposed to the alchemical approach (also known as combinatorial chemistry) of conducting zillions of experiments mixing things together and seeing what happened. We are entering an age when, like Vitruvius, we design the thing we are going to make, and then we make it. It is still a simple age, for we have not developed chemical equivalents of the architectural design methods and construction techniques of the Renaissance. That's what's coming next.

Meanwhile, the design of buildings has become divided between architects, who are theoretically concerned with the overall form and ergonomics of the building, while structural engineers are concerned with the integrity and soundness of the buildings. The growing demands on the actual performance of modern buildings -- to lower energy costs, reduce environmental footprints, enable ready navigation, etc. -- suggest that the demand for the mathematical tools for comprehensive design will only increase. And design considerations will include the geometry of the structure itself.

This web-page is not the first manifesto about reticular geometry, although it may be the first current one with a mathematical slant. For a more materials science slant, see:

- Building Units Design and Scale Chemistry, by Gérard Férey; published in the Journal of Solid State Chemistry in 2000.
- Reticular synthesis and the design of new materials, by Omar M. Yaghi, Michael O'Keeffe, Nathan W. Ockwig, Hee K. Chae, Mohamed Eddaoudi & Jaheon Kim; published in Nature in 2003.

The books to begin are probably:

- *Three-dimensional Nets and Polyhedra*, by Alexander Wells. This is the book that got crystallographers to look carefully at crystal nets.
- Crystal Structures I: Patterns and Symmetry, by M. O'Keeffe & B. G. Hyde. Probably still the basic source on crystal nets.
- *Quasicrystals and geometry*, by Marjorie Senechal. Overview.

Here are some links to scientific and engineering enterprises that are increasingly relying on reticular geometry for design, and to resources:

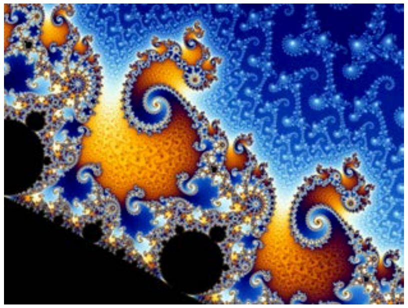
- The International Society for Nanoscale Science, Computation and Engineering.
- The Nanoengineer, "computational tools for structural DNA nanotechnology" produced by Nanorex.
- The Society of Industrial and Applied Mathematics has an Activity Group for Mathematical Aspects of Materials Science

Here are links to some resources specific to crystal design:

- Atlas of Prospective Zeolite Structures
- Cambridge Structural Database from Cambridge Crystallographic Data Center
- The Chemical & abstract Graph environment (CaGe)
- EPINET: Euclidean Patterns in Non-Euclidean Tilings
- The GAVROG Project, including the program SYSTRE

negatively charged components adhering to eachother without formal conjugal relationships comparable to covalent bonding (like sugar). If we want to model components fixed in position by potentials or stranger effects, we need some kind of geometric representation of the potential emerging from the assembled structure and then acting on that assembled structure.

As an example of the third direction, consider the problem of protein folding, in which one not only has a long chain of amino acids forming a peptide or protein, but then that chain wants to fold up so that "distant" acids on the chain will interact, distorting the structure further. The question is: what does the resulting structure look like? This is a computationally difficult problem, and at the moment (practiced) ad hoc human intuition seems to be more effective than contemporary algorithms: humans can practice their intuition folding proteins at the fold.it site. The question is: how do we compose a compact and usable mathematical description of what we see happening when we play fold.it?



Partial view of the Mandelbrot set, posted in Wikipedia Commons.

Another direction is the Chinese box problem: frequently, an intricate object (like a cathedral) will have intricate architectural elements (like flying buttresses) which may itself have intricate architectural elements (like gargoyles), and so on. The most popular mathematical example is the fractal, which was introduced in the early Twentieth century by Helge von Koch as a concrete example of a continuous but nowhere differentiable function; they were popularized by Benoit Mandelbrot, who sold many people, from biologists to cinematic special effects engineers, on the use of iterative processes to generate complex structures. In many ways, these fractals seem to be scratching the surface, for they do not seem to display the potential of, say, Matryoshka dolls to generate objects that vary depending on the scale. But the field is still rather new.

And then there is the issue of the effect that such structures have on their environment, e.g., the x-ray diffraction patterns one obtains when shining radiation of particular wavelengths through them...

Here are some books to start with.

- *Tilings and Patterns: An Introduction*, by Branko Grunbaum and G. C. Shephard. Still the primary source on tilings.
- *Groups, Graphs and Trees*, by John Meier. Introduction to geometric group theory on graphs.
- *N-dimensional crystallography*, by R. L. E. Schwarzenberger. Algebraic & analytic approach to the space groups.
- *Geometry and Symmetry*, by Paul Yale. Geometric approach to the space groups.

Here are some links & resources.

- The Association for Computing Machinery has a Special Interest Group on Graphics and Interactive Techniques (SIGGRAPH)
- David Epstein's list of Geometry in Action journals.
- Jeff Erickson's list of Computational Geometry journals, and his Computational Geometry links.
- Jemanshu Kaul's list of Journals (etc.) in Discrete Mathematics and related fields
- Jon McCammon's page of links for Geometric Group Theory
- The Society for Industrial Mathematics has a Special Interest Activity Group on Geometric Design

- GRINSP: Geometrically Restrained Inorganic Structure Prediction
- MathCryst: Commission on Mathematical and Theoretical Crystallography; International Union of Crystallography
- Nanorex, home of the Nano-engineer program
- The U.S. Navy's crystal lattice structure site.
- Reticular Chemistry Structure Resource [RCSR]: A database of extant nets, layers, and polyhedra
- USF's own Smart Metal-organic Materials Advanced Research and Technology Transfer (SMMARTT) interdisciplinary research center.
- TOPOS: Topological Classification of Nets
- S-window Crsytalline Structures and Densities (SCrysDen)

The Sociology of Reticular Geometry

The careful reader of this web-page will notice something weird about reticular geometry: it has been in near continuous demand for at least two millennia, almost certainly at least four or five, and probably much longer. And yet *academics* -- i.e., the participants in the system of subcultures of scholarship and learning -- have at best dabbled in it on occasion. The near silence in the respectable literature -- in ancient Greece, there is a thread on highly symmetric polygons and polyhedra from Pythagoras to Archimedes and that's all -- may lead an incautiuous observer to conclude that reticular geometry was invented one bright sunny morning by Johannes Kepler.

Tiled floor in Herculaneum, from Wikipedia Commons.

Yet the appearance of highly (and often accurately!) articulated structures from the Pyramids to the Pantheon suggest that either there was an academic tradition of reticular geometry that has been lost (quite possible!), or that there was a folk geometry practiced by architects and engineers that attracted little attention from scholars (also quite possible, recalling snide scholarly comments about engineers). Or perhaps something in between.

And of course, today there is a great deal of interest among computer scientists in computational geometry, which may correspond to the interest ancient engineers had in the subject. Computer scientists are also interested in the artistic and illustrative uses of computer graphics, which is used widely by engineers modelling their intended products.

Still, the inattention from mathematicians has been enough to irritate crystallographers into all sorts of public grumps, like the protests (see the ScienceBase post on Nature's Missing Crystal -- Found It!) that met the publication of Toshikazu Sunada's article in the AMS Notices on Crystals That Nature Might Miss Creating; the publication of a feature article in a mathematics flagship, a feature that overlooked a stream of literature in materials science, was treated almost as an offense instead of a goof. This hypersensitivity by the materials scientists suggests a certain unhappiness with academic mathematicians. Of course, materials scientists are not the only ones to whine about mathematicians, and in fact this kind of situation is not even unique to mathematicians. For example...

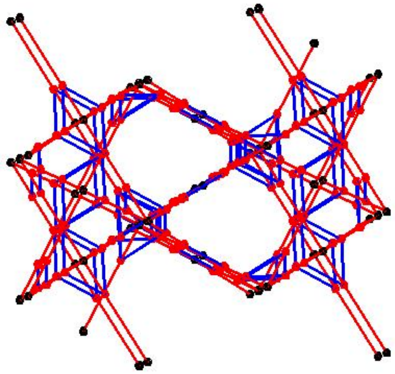
The traditional view of paleontology was that it was launched in the Renaissance when Europeans like Leonardo da Vinci started finding strange fossils -- in Leonardo's case, sea shells on mountainsides. But recently, folklorist Adrienne Mayor has found a lot of evidence of interest in and theorizing about fossils in Antiquity, suggesting that there was a sort of folk or proto-paleontology back then -- a proto-paleontology that may have been ignored by respectable biologists in Antiquity.

This kind of situation has recurred many times in the history of science. Reticular geometry seems to have had a similar experience within the mathematical community itself.

One complicating factor is the peculiar position of geometry in mathematics, science, and the community at large. While polyhedra have provided some of the primary symbols of mathematics to the lay public, and while geometry has long been a foundation of science, it's centrality to mathematics has declined since

My Adventures in Reticular Geometry

I was originally trained in mathematical logic, in particular finite model theory, and I also dabbled in combinatorics and applied probability, but after being abducted by chemists, I started working on the problem of designing crystals that chemists could synthesize. I have worked on programs that would design crystals, and these led me to the theoretical issues underlying the programs, and thus directly into reticular geometry.



My programs have found a lot of crystal nets, some already known, some new, some chemically plausible, some not. Image is output from my Maple program.

I got started with somewhat non-geometric but still reticular (articulation) issues in DNA computing, but gradually turned to crystal design using reticular geometry. During 2007, I worked with Edwin Clark on a heuristic to generate crystal nets (which in turn rests on the mathematical properties of periodic graphs), and he composed a program, based on a heuristic capable of producing nets from any isomorphism class of uninodal nets.

I have since developed a heuristic capable of producing crystal nets from all isomorphism classes, using techniques from geometric group theory and linear algebra, although the justification that it works requires some analysis. This heuristic is in the same family as the GRINSP and SCIBS heuristics, in that one starts with a putative fragment of the net and applies a symmetry group to that fragment to get lots of fragments that together make up the entire net. In practice, I have a sort of Model A contraption that has given me lots of binodal (two orbits of vertices) nets of one or two orbits of edges; hopefully, successor programs under development will be more powerful.

Meanwhile, I am trying to understand reticular geometry as a field in itself, which includes getting an idea of what it's theoretical structure looks like. All input on this exploration is welcome (my email address is mccolm@usf.edu).

Announcements

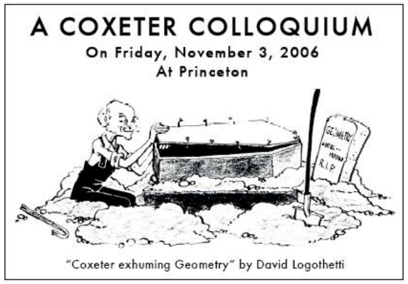
Two things:

- An extremely hostile Version 0.8 of the Crystal Turtlebug program has been posted at Sourceforge. It consists of several Python worksheets, and input is via a Python worksheet. We are working on improving many aspects of the program, including I/O. Comments are appreciated.
- I am putting up a new Crystal Mathematician weblog and web resource. Comments are appreciated.

My Research

Newton; while geometry and number theory were the pillars of mathematics up into the Renaissance, that was not true afterwards, no matter what Kant said about space (geometry) and time (number theory), and by the Twentieth century, the pillars of mathematics were algebra and analysis.

The appearance of non-Euclidean geometries and their applications to science (especially in the theories of relativity and quantum mechanics) seems to have led to geometry, *as a social phenomenon*, being more about *space* than about *constructions in space*. Of course, artistic movements were inspired or partly inspired by geometry were interested in things in space, and chemists and materials scientists doggedly concentrated on things in space, so geometric constructions continued to appear. Artists like Maurits Cornelis Escher and mathematicians like Harold Scott MacDonald Coxeter continued to be interested in the shapes of things *in* space.



David Logothetti's cartoon of "Donald" Coxeter exhuming geometry, posted in a PDF by Steven Cullinane.

Some mathematicians are interested in the shapes of things in space, although much current research on constructions like buildings is aimed at finding accessible representations of groups: so again, much of reticular geometry in mathematics is in service to algebra, and its service is to make geometric representations of algebraic objects. This is not unlike the service that reticular geometry provides for computer graphics and geometric design (modelling), but the result is that there is relatively little "pure" reticular geometry.

A lack of pure reticular geometry translates into a lack of pure reticular geometers, but on the other hand, the fact that reticular geometry pervades several domains outside of mathematics departments was seen at two conferences.

- In April, 1984, at Smith College, elementary school, middle school, high school, college and graduate students, teachers, artists, scientists, mathematicians, engineers, architects, model-building enthusiasts, mystics and townspeople attended a *Shaping Space Conference*, from which Marjorie Senechal and George Fleck derived the anthology, **Shaping Space: A Polyhedral Approach**.
- In November, 2007, at the University of South Florida, participants spent several days Knotting Mathematics and Art: Conference in Low Dimensional Topology and Mathematical Art. Artists, mathematicians, and nanoscientists discussed very similar objects.

And it doesn't take much effort to find all kinds of polyhedral and even stranger articulating structures in graphics scattered about the www.

Meanwhile, scientists and engineers do all kinds of reticular geometry -- without mathematical supervision. Just as the High Culture world distinguishes between arts (like painting and sculpture, practiced by artists) and crafts (like jewelry and apparel, practiced by craftspeople), so there seems to be a distinction between mathematics produced largely by mathematicians, and ("folk"?) mathematics produced largely by non-mathematicians. Much of reticular geometry may fall in the latter category.

Here are some enthusiasts, scholarly or otherwise:

- David Eppstein is a professor of computer science at UC Irvine, and maintains a Geometry Junkyard.
- George Hart is a sculptor, and he maintains an on-line Virtual Polyhedra: Encyclopedia of Polyhedra.

Probably the places to begin are the two Wikipedia pages that I launched:

- Periodic graphs (geometry) goes into models of crystals (at the molecular or atomic level) from a mathematical point of view.
- Periodic graphs (crystallography) goes into the project of using these models to analyze or even design crystals.

I also wax eloquent on mathematically crystallographic matters on my new weblog as the Crystal Mathematician. My primary project is:

The Crystal Turtlebug

The Crystal Turtlebug crystal design program posted on Sourceforge generates blueprints for designing crystals at the atomic or molecular level.

Then here are some papers ... more on the way.

- Here is my talk on the heuristic presented to the Forty-First Southeastern International Conference on Combinatorics, Graph Theory, and Computing conference in Boca Raton, and here is the communication announcing the program in Crystal Growth and Design.
- Conference papers for which the main papers are being composed:
    - A Computational Model for Self-assembling Flexible Tiles (with Natasha Jonoska) **4th International Conference on Unconventional Computation**, Sevilla, Spain, October 2005, in: **Proceedings LNCS 3699**; ed. by Cristian S. Calude, Michael J. Dinneen, Gheorghe Paun, Mario J. Prez-Jimnez, Grzegorz Rozenberg; pp. 142 – 156.
    - Flexible versus Rigid Tile Assembly (with Natasha Jonoska) **5th International Conference on Unconventional Computation**, York, England, September 2006, in: **Proceedings LNCS 4135**; ed. by Cristian S. Calude et al; pp. 139 – 151.
    - Describing Self-assembly of Nanostructures (with Natasha Jonoska) **SOFSEM 2008: Theory and Practice of Computer Science** Novy Smokovec, Slovakia, 2008, in: **Proceedings LNCS 4910**; ed. by Alberto Bertoni, et al; pp. 66 – 73.
    - A Formal Crystal Description System (with W. E. Clark and M. Eddaoudi), presented at the 2008 ISNSCE Foundations of Nanoscience (FNANO) Conference.
- Main papers:
    - The group-theoretic formulation of the algorithm is described in Generating Geometric Graphs Using Automorphisms.
    - The module-theoretic formulation of the algorithm is described in Periodic Euclidean Graphs on Integer Points.
- On the related area of DNA computation:
    - *Complexity Classes for Self-Assembling Flexible Tiles* (with Natasha Jonoska), **Theor. Comp. Sci. 410:4-5** (2009), 332–346.
    - *On Stoichiometry for the Assembly of Flexible Tile DNA Complexes* (with Ana Staninska and Natasha Jonoska) **Natural Comp. (2010)** (20DOI: 10.1007/s11047-009-9169-1).