A MATERIAL GEOMETRY KERNEL FOR COMPOSITE AND BIOMATERIALS

Edward L. Stanton
MSC.Software Corporation
2 MacArthur Place
Santa Ana, CA 92707

Abstract - The DNA schema with four primitives (the nucleotides) and 64 elements (the codons) is intriguing for many reasons. One is the taxonomy, which is very similar to that of a schema used for the solid modeling of composite materials. It also has four primitives, the four cubic Hermite polynomials, and 64 elements, the tricubic Hermite polynomials called hyperpatches. Each system creates material objects from their respective primitives. In both systems there are different "genomes" that map the primitives into specific material objects with specific structures according to their function. In biomaterials the expression of the DNA schema begins with the amino acids of which there are only 20 but they can be combined mathematically to form more proteins than there are atoms in the known universe. These are the building blocks of virtually all biomaterials.

In hyperpatch models the primitives have only four possible base pairs because the end points and the end point slopes must connect to each other to avoid mixing geometric functions. The DNA schema also has only four possible base pairs of the four nucleotides, AT, TA, GC and CG. At this level the taxonomy's match exactly. At the next level, however, the 64 codons map to just 20 amino acids [1], and here the taxonomy begins to get complicated. How the DNA taxonomy at this level relates to the hyperpatch taxonomy remained a complete mystery for many years until combinatorial methods were used. In combinatorial math the number of combinations of 4 things taken 3 at a time with recurring elements counted once is (4+3–1)! / 3!(4+3-1-3)! = 20 and that is used in this paper to relate the taxonomies at this level, Figures 1-2. Nevertheless taxonomy differences persist including how the three stop sign codons [2], TAA, TAG, TGA can be related to hyperpatch codons.

The duality of the material models is of interest for many reasons. Both use "bottom-up" methods [3], to build material objects from their respective primitives into macro material objects. This is the opposite of sculpting an object from a monolithic block of material. Composite materials and many biomaterials have skeletons of reinforcing fibers or trabeculae whose architecture is determined by their function. Can the material geometry models developed to represent composite material behavior be used for biomaterials? This paper explores a related question using carbon nanotubes that like biomaterials self-assemble at the atomic level. The two assembly processes and environments are very different but the same material geometry kernel may describe the anisotropic behavior of both.

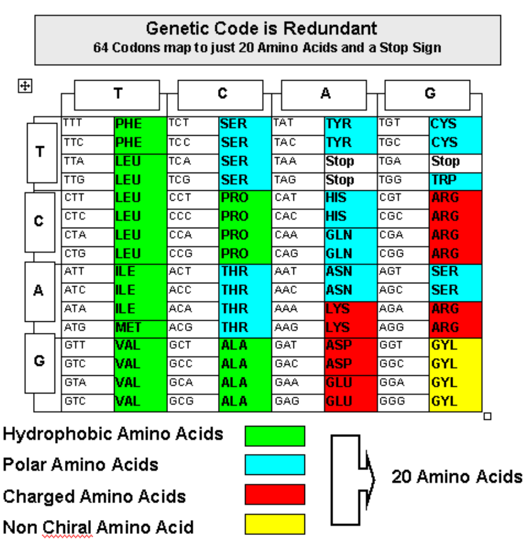

Figure 1. DNA Genetic Code Taxonomy

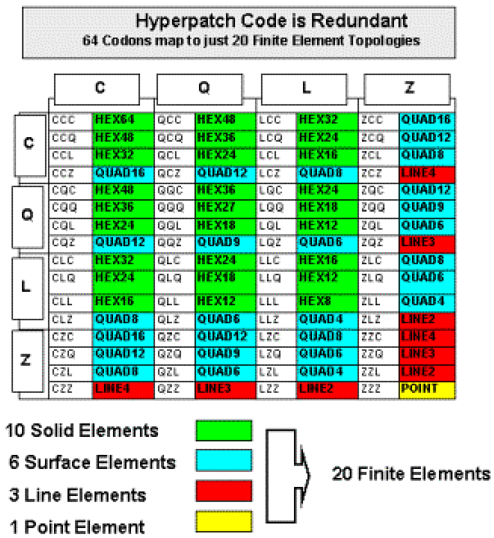

Figure 2. FEM Hyperpatch Taxonomy

Composite Material Geometry Overview

In Mechanical Engineering the term composite material usually refers to one of three classes; a polymer matrix, ceramic matrix or metal matrix composite often abbreviated as PMC, CMC and MMC. By material geometry we mean the spatial distribution and orientation of the reinforcing and matrix materials in a Unit Cell. Normally these are modeled as solids or shells and the scale of Carbon fiber diameters is on the order of a millimeter. Today material geometries at the nanometer scale are appearing in production applications and we start the overview with the stable forms of Carbon.

Carbon Fullerene and Nanotube 1-D Geometry

The isomers of Carbon, Table 1, are unique in that Carbon is the only element in the periodic table with isomers of dimension 0,1, 2, and 3. The fullerenes and nanotubes are fairly recent discoveries that have sparked a nanotechnology explosion in the material sciences, Figure 3.

Table 1. Isomers of Carbon*

Dimension	0-D	1-D	2-D	3-D
Isomer	C60 Fullerene	Nanotube	Graphite	Diamond
CC Bond Length	1.40-6 A°	1.44A°	1.42-4A°	1.54A°
Density [g/cm^3]	1.72	1.2-2.0	2.26	3.515

*Physical Properties of Carbon Nanotubes, 1998 [4].

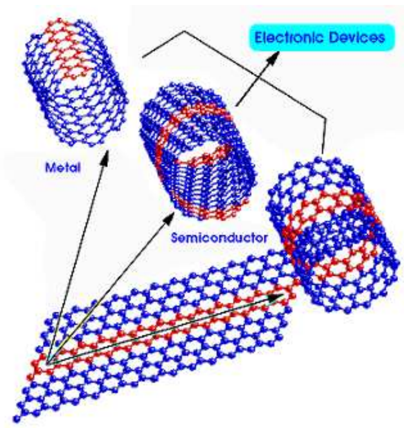

Figure 3. NASA Computational Nanotechnology Project

The geometry of nanotubes is defined by the chiral vector (n,m) with (5,5) being the smallest (n,n) nanotube [4]. Two of the isomer geometries are illustrated in Figure 4 showing a single walled (5,5) carbon nanotube with a C60 fullerene cap formed from pentagons and hexagons. As Smalley noted [5], the C60 fullerene has the shape of a truncated icosahedron discovered about the time of Archimedes.

At this scale only the simplest geometry elements are needed to create a finite element model for mechanical analysis, Figure 5. In this case the ZZZ (Point) and ZZL (Line 2) entities from Figure 2 define both the material geometry and the FEM geometry. For this example Saito's code [4], was used to compute Unit Cell Carbon coordinates. Each atom is connected to its three nearest neighbors. The atomic level physics models that determined the lattice constant dimensions were not required to compute the Unit Cell coordinates for the nanotube finite element model.

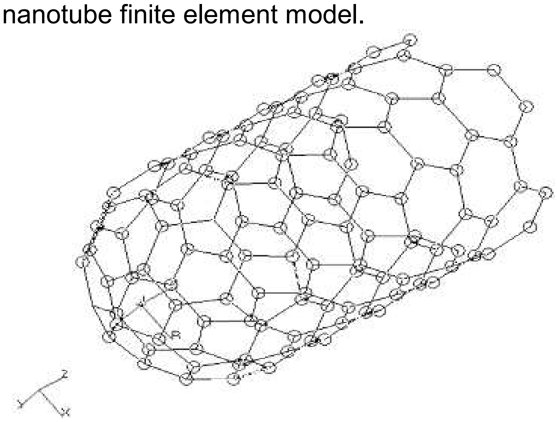

Figure 4. C60 Fullerene Cap on a (5,0) Carbon SWNT FEM Model

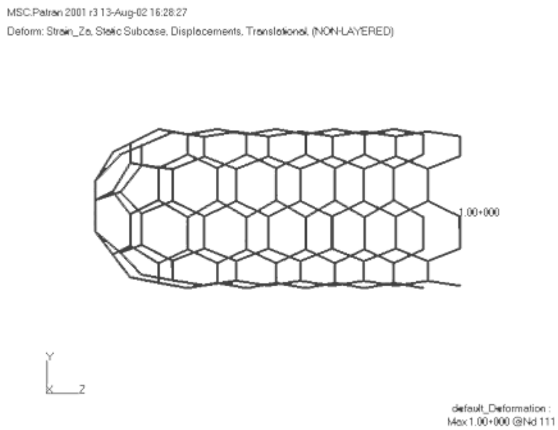

Figure 5. C60-SWNT (5,0) FEA Results – Tensile End Load

The Cap contains 30 Carbon atoms, one-half of a C60 Fullerene, and was created using 6 pentagons and 10 hexagons. The C-C bond length of the pentagons is exactly the same as the hexagons. One-half of a planar template for a truncated icosahedron was mapped to form the Cap. Each hexagon and pentagon was translated and rotated about a local C-C bond line, a folding operation, to create the Cap seen in Figure 4. The template is analogous to a "Cap gene" and a conformal map of the planar template forms the cylinder Cap in a process analogous to gene expression.

The (5,5) nanotube Unit Cell contains 20 carbon atoms [4], and that Unit Cell was translated 4 times to form a tube with 100 atoms. The two components were assembled (docked) at the 10 points where they have a carbon atom in common to form a finite element model with 120 nodes. Note that the cap geometry is "exact" meaning the C-C bonds are unstrained. The nanotube, however, is strained by the curvature of the cylinder and has a slightly larger C-C bond length, Table1, in order to mate with the Cap. The 120 atom model was subjected to a uniaxial strain by restraining the 5 nodes that form the pentagon top of the Cap and imposing a unit axial (Z) displacement on the 10 atoms at the free end of the nanotube, Figure 5. In effect a symmetry boundary condition.

A single template approach to modeling a capped (n,m) nanotube is also possible. Asimov [6], explains how this can be done by mathematically cutting six 60-degree darts in a planar graphite sheet. That template is folded or draped onto the reference capped cylindrical surface to create a (n,m) nanotube model. Each end cap will have six pentagons and the rest of the model will be hexagons. A good introduction to the physical properties of Carbon nanotubes and how composite nanostructures are created in the laboratory can be found in the book by Saito, et. al. [4]. In that work connections between Carbon nanotubes of different diameters were created in the lab and models of the transition (conical) created using pentagons, hexagons and heptagons.

The purpose here is to demonstrate that a FEM beam model can simulate the elastic response observed in molecular force probe measurements of end loaded Carbon nanostructures. This is to be expected after the work of Gao and others [7]. First a unit stretch of the nanotube FEM beam model without the end cap produced a Poisson ratio of 0.28 in agreement with Lu's results [8]. His force-constant model uses pairwise harmonic potentials between atoms. This indicates the FEM elastic response simulation is correct at this level. Next the end cap was attached to the model and a unit stretch of the capped nanotube model produced a much smaller Poisson ratio of 0.06, a value between the Poisson ratios of graphite in the basal plane and C axis [7]. This result seems reasonable but needs to be checked using an empirical force-constant model which is beyond the scope of this paper. Other loads and boundary conditions (LBCs) were tested, Figure 6, during testing on a variety of Carbon nanotubes. These beam models capture the strong covalent bond behavior under strain. A multilayer nanotube would require modeling the weak van der Waals bonds as well and that's much easier to do using shell finite elements.

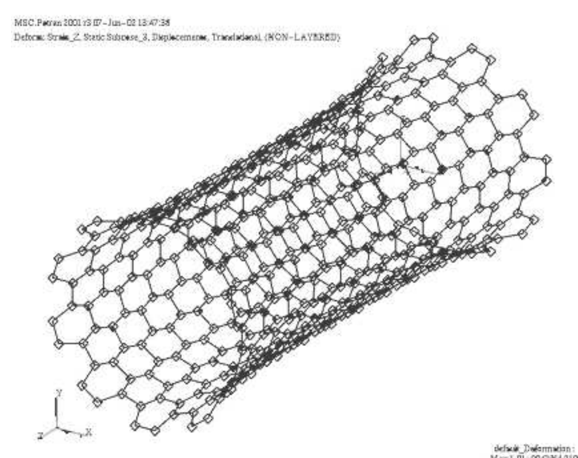

Figure 6. Carbon SWNT (10,10) FEM Model LBC Testing

Carbon Nanotube 2-D Surface Geometry

As interesting as these beam models of nanotubes are, there is arguably more interest in continuum shell models for nanostructures because of the greatly reduced number of degrees of freedom needed to scale up to multi-walled nanotubes and beyond. This is where the material geometry and structural geometry become distinctly different. Here the FEM model geometry usually conforms to spherical and cylindrical coordinate frames. The material geometry conforms to the twist or chirality of the graphite hexagons relative to the tube axis. This is like modeling the ply orientation of a bias ply in a laminated shell structure. It is important in shell models that inter-element fiber continuity and fiber orientation continuity be maintained to accurately model the shear behavior of composite materials.

This is where the Hermite polynomials have a special role to play. Instead of the algebraic form; C, Q, L, and Z, we need the Hermite form of the four polynomials to connect fibers in our model with slope continuity. This is a simple linear transformation of the polynomial coefficients that makes the polynomial end points and their slopes the control parameters for assembly. The transformation matrix is shape-independent [9], and can be applied to line, surface and solid models. Mortenson [10], provides a well-illustrated introduction to Hermite polynomial models for parametric cubic lines, bicubic patches and tricubic hyperpatches. His focus is the external shape representation of continuum objects.

These were the math models used in the original Patran hyperpatch finite element solid modeling system [11], to represent material geometry. Here the chiral angle for a nanotube is constant but in general material orientation various over the lay-up surface of a composite shell structure. At each continuum material point a material orientation angle is needed to generate the stiffness matrix for a finite element with inter-element material orientation continuity, Figure 7. A bicubic kernel can define the local material axis orientation at any point in any finite element in the support region [12], of the kernel. The kernel support region can be as small as a single element or as large as the entire shell in some cases depending on how nonlinear the fiber direction changes are over the shell surface. The use of the kernel decouples the finite element meshing process from modeling material geometry.

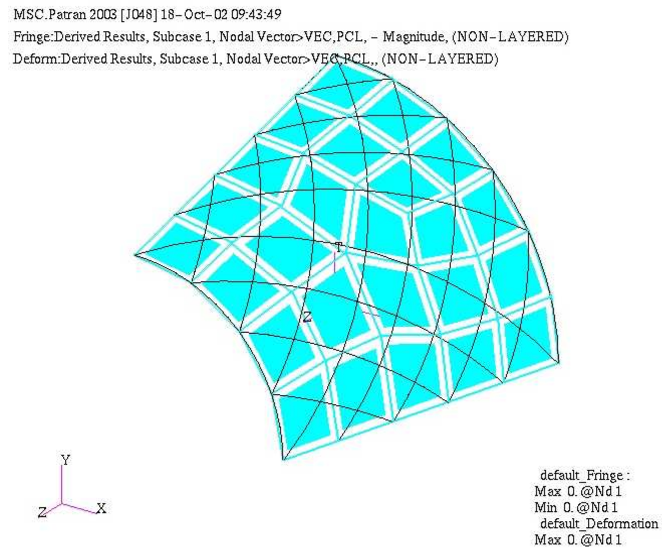

Figure 7. Bicubic Material Geometry Kernel for a Shell Elements

Laminate 3-D Solid Geometry

A material orientation service is even more important for 3-D finite element models. In the case of a simple thick laminate 2.5-D construction this is an extension of shell composite modeling. In the case of a general 3-D material geometry, the kernel must provide three material angles [11], to define variable fiber orientation throughout the volume of the structure. The finite element hyperpatch solid modeling system creates tricubic representations for fiber orientation derived from representations of the composite manufacturing process that actually controls fiber placement. Again we decouple meshing from material geometry relying on the kernel to provide a 3-D material orientation services.

An early industrial application of hyperpatches was for laminated involute composites, Figure 8, used in Carbon-Carbon rocket motor nozzles. The ply surfaces spiral out from the interior nozzle surface to the exterior surface. This is the only constant thickness ply shape that fills a conical volume exactly with ply edges on the interior and exterior surfaces. This geometry is difficult to describe analytically and illustrates the role of a material solid geometry kernel in generating a finite element structural model.

How the three Euler angle rotations at each material point are determined from the ply pattern template is available [13], and the details are not presented here. The important point for this work is that the material geometry for the 3D finite element model was represented by a CQLZ tricubic hyperpatch.

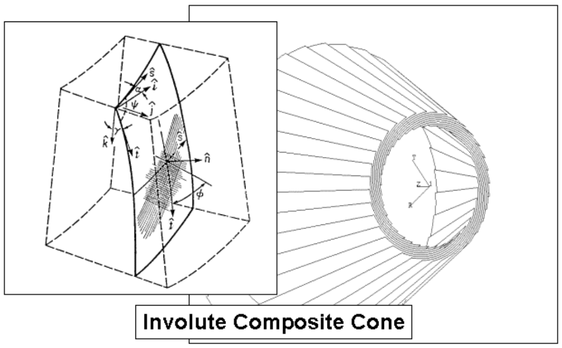

Figure 8. Tricubic Material Geometry Kernel for Solid Elements

Conclusions and Recommendations

This paper shows that the taxonomy of the CQLZ hyperpatch material geometry kernel used for composite materials is the same as that of DNA for biomaterials and asks the question can the CQLZ kernel be used for biomaterials. The paper examples addressed a simpler question, can the CQLZ hyperpatch material geometry kernel create finite element models for Carbon nanostructures. At this point we are at the working hypothesis stage for simple molecular structures. We were able to create capped Carbon nanotube models from ZZZ and ZZL templates for the C60 cap and the C20 Unit Cell of a (5,5) nanotube and other nanotubes. The templates were conformally mapped to the capped nanotube surface using translations and rotations only. Beam finite element tensile load simulations of a single walled nanotube's elastic behavior were used to test the model for a single parameter, Poisson ratio, and that result was in good agreement with Lu's simulation data. This is hardly a validation of the finite model but it is a promising result. The choice of Carbon nanotubes for this study is a reflection of the author's interest in Carbon based materials more than anything else. The modeling of other nanocomposites and protein structures using the CQLZ kernel would make an interesting research topic. A topic not discussed here is an "RNA" expression of the CQLZ kernel. We associate that function with the Hermite form of the kernel in the taxonomy metaphor.

Recently in a University laboratory the DNA of biological materials were used to control the assembly of inorganic nanostuctures. This paper suggests ways the coevolution of organic and inorganic materials may work together in the sense that Stuart Kauffman [14] uses to describe biological and technological coevolution. Carbon nanotubes that were first thought limited to nanostrutures have recently been produced as continuous yarn of pure carbon nanotube fiber 30 cm in length at a University in China [15]. Models capable of representing material geometry at every scale from nanometers to meters are going to be needed, especially when self-assembly is required to create a nanoscale structure.

Acknowledgements

The author would like to thank all the many colleagues over the years whose work helped contribute to the CQLZ hyperpatch material geometry kernel for composite materials. These include lifelong friends in Nasa, the DoD, Douglas Aircraft, McDonnell Aircraft, Boeing, PDA Engineering and MSC.Software. These also include the many University colleagues and other professionals that I have collaborated with in AIAA, ASC, ASTM, NIST and ISO committees.

References

[1] C. Branden & J. Tooze, *Introduction to Protein Structure*, Garland Publishing, Second Edition, [1999].

[2] P. Pevzner, *Computational Molecular Biology*, MIT Press, [2000].

[3] N. Seeman & A. Belcher, *Emulating Biology: Building Nanostructures from the Bottom Up*, Proc. Natl. Acad. Sci. USA, Vol. 99, Issue 90002, April [2002].

[4] R. Saito, G. Dresselhaus & M. Dresselhaus, *Physical Properties of Carbon Nanotubes*, Imperial College Press, [1998].

[5] R. Smalley, *Discovering the Fullerenes*, Reviews of Modern Physics, Vol. 69, No. 3, July [1997].

[6] D. Asimov, *Geometry of Capped Nanotubes*, AT&T Labs Research Paper, November [1998].

[7] G. Gao, T. Cagin, & W. Goddard, *Energetics, Structure, Mechanical and Vibrational Properties of Single Walled Nanotubes (SWNT)*, Fifth Foresight Conference on Molecular Nanotechnology, [1997].

[8] J. P. Lu, *Elastic Properties of Carbon Nanotubes and Nanoropes, Physical Review Letters*, Vol. 79, No. 7, 1297-1300, [1997].

[9] E. L. Stanton, *Geometric Modeling for Structural and Material Shape Optimization*, The Optimum Shape, Plenum Publishing, [1986].

[10] M. E. Mortenson, *Geometric Modeling*, John Wiley & Sons, New York, Second Edition, [1997].

[11] E. L. Stanton, L. M. Crain & T. Neu, *A Parametric Cubic Modeling System for General Solids of Composite Materials*, Int. Jour. Num. Meth. Engng., Vol. 11, [1977].

[12] T. Hastie, R. Tibshirani, & J. Friedman, *The Elements of Statistical Learning*, Springer-Verlag, New York, Corrected Printing [2002].

[13] J. K. Hart, E. L. Stanton, & L. A. Schmit, *Material Geometry Optimization of Involute Structures Using Sensitivity Derivatives with Respect to Global Design Variables*, AIAA/ASME/ASCE/AHS/ASC 31st Structures, Structural Dynamics and Materials Conference, pp. 356-370, [1990].

[14] S. Kauffman, At Home in the Universe: *The Search for Laws of Self-Organization and Complexity*, Oxford University Press, [1995].

[15] K. Jiang, Q. Li, & S. Fan, *Spinning Continuous Carbon Nanotube Yarns*, Tsinghua University, Nature, Vol 419, October [2002].