

# FROM BIOLOGICAL MACROMOLECULES TO DRAPE OF CLOTHING: 50 YEARS OF COMPUTING FOR TEXTILES

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## INTRODUCTION

### Historical

With a few years overlap at each end, the second half of the 20<sup>th</sup> Century has seen the rise of computing, as indicated below, and the study of the structural mechanics of fibres and fibre assemblies – as well as coinciding with the professional career of the presenting author (jwsh). An account of the history is instructive, but more attention will be paid to matters of current concern, particularly the TechniTex core research in the University of Manchester on the modelling of woven fabrics and the work of jwsh with Canesis Network Ltd (formerly Wool Research Organisation of New Zealand) on wool and hair. The paper will progress from the nano-scale of molecular structures, through the micromechanics of fibres, yarns and fabrics, to the macromechanics of overall performance of products. The level of computation in each study is indicated by comparison with the dates in the following list, for which some poetic licence has been taken in order to present a simple story.

- 1950: First programmable computer had been built by Williams and Kilburn in Manchester. Major users only – programmed by changing switches.
- 1960: Batch processing by punched cards. Answers in hours to days. First languages. Mercury and Atlas code in Manchester to Fortran by IBM.
- 1970: Batch processing by teletype input.
- 1980: On-line from terminals to main-frame computer.
- 1990: Personal computers. Advanced languages. Powerful graphics.
- 2000: Global interaction by internet and e-mail.

In reality, each development ranged over several years, with people and places being at different stages. For example, in July 1967, we made an on-line trans-Atlantic connection through the commercial telex network from Manchester to the textile information retrieval system on a computer at MIT, but it was many years later and with new technology before this became commonplace. Around this time, the Professor of Computing at UMIST saw no place for anything but batch processing on large main-frame computers, but the Professor of Control Engineering was pioneering on-line access to a PDP 10 mini-computer. *Milos Konopasek* used the PDP 10 for innovative computing techniques for textiles, but it is only now that there is a prospect of industrial usage.

### Routes to follow

In the beginning, we used computers as little more than powerful calculators to carry out the sums at the end of an investigation. Later it became common practice to carry out complex mathematical analyses and use computing routines for numerical evaluation at the end of the

study. Alternatively attempts were made to apply techniques, such as finite element methods, that had been developed in other contexts. Because of the nonlinearity and complexity of textile systems, these academic routes seem doomed to failure as quantitative design tools. For software that will have industrial application, one should start by considering how computing can best deal with the fundamental relations governing a fibre system and how, in a way that is easy to use, it can give useful answers. Getting the right software into industrial use is a necessity, in order to bring about the creative interchange between researchers and users, which has so far been lacking.

Prejudice has to be overcome. The textile industry has an amazing history of empirical development, but the triumph of the practical advances breeds a reluctance to embrace computer-aided design. There are two areas where there were great changes in the last quarter of the 20<sup>th</sup> Century. One was in computer control of machines, typified by electronic Jacquards and complete production of 3D garments by flat-bed knitting. The other is more relevant to this paper and can be illustrated by a Manchester story. In 1975, textile designers did not like the idea of using computers for the aesthetic design of fabrics by colour and pattern. An earlier grant application by UMIST and the Royal College of Art had failed because it was said that “why do designers need computers, they have pantographs?”. *Peter Grigg* was appointed a Lecturer in Textile Engineering; he obtained Elliot 903 computers, which were the size of upright pianos and thousand of times less powerful than a modern PC, that were no longer needed by the Navy, and developed a textile CAD system. In the 1980's, TCS Ltd was formed to exploit the system; in the 1990's, the company was bought by Ned Graphics, who now have large stands at textile machinery shows. In this aspect of textile design, the use of CAD is universal. The same is not true of the engineering design of fabrics. For technical textiles, qualitative trial-and-error, backed by experience, is the norm. One challenge for the 21<sup>st</sup> Century is to exploit the academic work of the last 50 years and bring in CAD; another is to advance the methodology, stimulated by a creative interchange between industry and academia.

### **Approaches to mechanics**

There is one more general point to make. The first approach to modelling textile mechanics has usually been to apply equilibrium of forces and moments. However, almost always, energy methods have proved more powerful. There are various reasons for this, but the most basic is that forces and moments are vector quantities, so that equations are needed for six components. Energy is a scalar quantity, so that there is one basic relation to satisfy. If there is a geometrical relation between macro- and micro-strains, e.g. affine deformation, conservation of energy can be used; if the deformation is undefined, as in buckling, minimum energy or the principle of virtual work is used.

### **Space limitations**

Space does not permit a full listing of references. Instead, the names of those involved will be noted. Those in *italics* are associates of *jwsh*; details can be obtained from [johnhearle@compuserve.com](mailto:johnhearle@compuserve.com).

Limitations of space also prevent the inclusion of diagrams that would make the information easier to understand. Pictures will be included in the conference presentation and in any extended publication.

## MOLECULES TO FIBRES

### Wool and hair

Wool and hair have the most complex of fibre structures, with nine levels from atoms through a collection of proteins to the whole fibre. Table 1 is a simplified list of levels having most influence on properties. The stress-strain curve has Hookean, yield and post-yield regions and, surprisingly, full recovery from large strains, but along a different curve. It is explained (*Chapman, 1969*) as a composite of intermediate filaments, characterized by critical and equilibrium stresses for a phase transition with 80% extension, and a rubbery matrix. This model was so simple as not to need computation. Fortran programs covered more detail of filament/matrix interactions. Later, a BBC Acorn microcomputer was used to add time dependence to the model (*Susitoglu, 1985*). More recently, at WRONZ, buckling into crimped forms has been programmed (*Munro, 2000*).

Table 1. Important structural levels in wool and hair and relevant mechanics.

intermediate filament	matrix		stress-strain curves
↓ parallel assembly ↓			parallel composite
axial macrofibrils ↓	helical macrofibrils →		“twisted yarn”
para-cortex	ortho-cortex	cuticle	multi-component
whole fibre: tensile			parallel mixture law
whole fibre: bending, twisting,			rod and beam theory
whole fibre: crimp			differential contraction

Several computational advances are now needed. The previous work is simplified and generic. This gives scientific understanding, but programs should explore the differences, particularly if genetic engineering is used to modify structures. A full model should take outputs from one level as inputs to the next level (*Hearle, 2003*). Some parts of the total model, e.g. a simple dependence on mixture laws, are easy to program. Others are more challenging. At the nano-scale level, computational molecular modelling should be used to determine the full mechanical response of the complex protein assembly in intermediate filaments. The full repeat length is too large to compute, but it should be possible to model separate simpler segments and then link them in a series model. The matrix presents a greater problem, because, although it is critical in determining mechanical properties, its structure is less well known. The development of computational modelling would stimulate an interchange with molecular biologists. For the ortho-cortex, the methodology of twisted yarn mechanics needs to be extended to a system in which the matrix contracts on drying, with a consequent shortening of the macrofibrils. At the fibre level, the different properties of para-cortex, ortho-cortex and cuticle (sometimes also meso-cortex and medulla) need to be combined to predict bending, twisting and crimping modes.

### Other fibres

For all fibres, the fine structure has a major role in determining properties, but it has never been engineered deterministically, in the way that both molecules and macroscopic structures are engineered. For cotton and other plant fibres (*Sparrow, 1975*), with structures determined by nature, there are helical models. In the production of melt-spun fibres, fluid and heat flows are computed, but changes in structure result from “twiddling the knobs”. To predict properties, unpublished software (*Du, 1985*) included two useful features: the fine structure

was modelled by a collection of chains emerging from a crystallite; the energy was the sum from extension of tie-molecules and change of volume. There are challenges for advances in computational modelling, both of formation and effects of structures.

## **YARNS**

### **Twisted continuous filament assemblies**

Twisted continuous filament yarns have a well-defined geometry. Affine deformation relates yarn strain to fibre strain through helix angles. In the 1960's it was found the force-equilibrium analyses, which were limited to small strains and linear elasticity, were overtaken by large-strain, nonlinear energy methods introduced by Treloar and Riding. This gave a few easily programmed equations (Hearle, 1965). Torsion and plied yarns were later included (Konopasek, 1970). Development of these methods led to a first use in engineering design by a manufacturer. *Fibre Rope Modeller* (Leech, 2000) takes account of the multi-level structure of ropes. The basic yarn stress-strain curve is input through a set of polynomial coefficients. An earlier DOS version for the US Navy was converted to WINDOWS. In order to determine internal forces, which cause fibre fatigue, the principle of virtual work was used.

### **Other yarns**

For false-twist textured yarns, minimum energy computations of the various forms of alternating helices and pig-tail snarls have been carried out (Yegin, 1970). For air-jet textured yarns, the entanglements and loops were modelled (Kollu, 1985). For the simplest staple fibre yarns, the effects of slippage at fibre ends need to be included (El-Sheikh, 1964). These academic studies provide a basis for further work, but more is needed for realistic predictions. Bulky staple fibre yarns have been much studied from Carnaby (1975) to Cassidy (2000), but serious difficulties remain. The underlying problem is that, to be of any value, computational modelling of the physics of yarn formation is needed. An open question is whether a global treatment is possible or whether to follow the detail of individual fibre segments.

## **FABRIC CONSTITUTIVE RELATIONS**

### **Woven fabrics**

Almost all the many papers on the mechanics of woven fabrics have used force-and-moment equilibrium, with Kawabata's saw-tooth model being the most successful. However, this again seems to be a cul-de-sac, with no outlet to more realistic geometries, large deformations, and nonlinearities. An energy method (Shanahan, 1978) is the way forward. Through UK DTI-supported technology transfer, this has been converted into WINDOWS-based software, *TechText CAD*, in a form for industrial use, which is being marketed by TexEng Software Ltd. Another program, *Weave Engineer* (Chen), provides a link to weaving machine settings and covers both hollow and solid 3D weaves.

The authors of this paper are extending this approach to deal with more difficult aspects of woven fabric mechanics. The aim is to determine constitutive relations, for a fabric subject to uniform strain. The biaxial deformation of a simple plain weave is defined internally by two axial displacements and one transverse displacement, which link an origin to three other control points. For more complicated weaves and for shear and bending, more terms are needed. The two requirements are to define the geometry and to minimize the sum of

extension, bending and flattening yarn energies. Yarn lengths between control points are directly defined. In order to give generality, we have defined bent yarn paths by B-spline interpolation. Twisting would need to be taken into account when yarns follow 3D paths. Yarn flattening has been unduly neglected in the past. Previous studies have used symmetrical, circular, race-track or lenticular geometries. Real fabrics show other asymmetrical shapes. We have adopted a general form, in which the shape is defined by the radial lengths at a series of angles round the yarn circumference.

Unless the fabric has been totally relaxed, the initial specification of a fabric will not be the minimum energy state under zero applied forces. The first step is thus to minimize the yarn energies to determine this state. There is a paradox here. The state under zero forces, although attractive as a mathematical origin, is poorly defined. It is easily shifted due to hysteresis or friction. It may be better to define a fabric reference state under small biaxial forces. For the determination of biaxial deformation, the potential energies of applied forces, given by products of force or moment and displacement, must be included. Instead of direct minimization, it is better to determine the state of internal minimum energy at two closely spaced deformations, and then to equate the energy difference to the work done by the applied force. There are still difficult questions for energy minimisation. Yarn extension energy is known from experiment or yarn modelling. In principle, yarn bending is well understood and bending energy is given by the product of bending moment and curvature. However, the bending stiffness changes from a high to a low value when the fibres start to slip past one another. There is a different response in free lengths between crossovers and contact regions where there is inter-yarn pressure. Furthermore, in the contact regions, curvature is determined by a combination of bending energy and the less well understood energy associated with change of yarn shape. A further complication is that yarn shape may change as it moves from contact to free zones.

Progress is being made by simplifying in two ways. The first is to carry out energy minimization with simplified geometries for yarn paths and yarn shapes, so that the minimization involves fewer terms. Having obtained an approximate solution, the minimisation can be refined with the full B-spline and yarn radii specifications. The second is to solve two extreme cases. For monofilaments and hard twisted yarns, we assume that there is negligible change of yarn shape, except through Poisson's ratio due to length change. The curvature in contact zones is then geometrically defined and only the shape in free zones results from the energy minimization. Very soft yarns deform until the free zone has disappeared, so that it is only necessary to consider the combined bending and flattening energy in contact zones. Further research will lead to ways of treating the following problems: structures between the two extremes; shear and bending deformations; and non-plain weaves, in which side-by-side flattening as well as crossover flattening will occur.

### **Other fabrics**

Plain knit fabric was modeled using a powerful bending curve program (*Konopasek, 1970*). However, this approach has the same fundamental problem as for woven fabrics, and analogous energy methods need to be developed. Bonded nonwovens were modeled by energy methods based on the orientation and curvature of a representative set of fibre elements (*Newton, 1967; Oszanlav, 1979*), but agreement with experiment was only achieved by the input of measured values of lateral contraction and empirical rules for bond breakage. For needled fabrics, the model added in friction and fibre paths round transverse tufts (*Purdy, 1972*). Individual fibre computation will be needed for advances in modelling of nonwovens.

## FABRIC DRAPE

Early modelling of fabric drape showed its dependence on both bending and shear properties (Cusick, 1962). It is the low resistance to shear and area change, that gives weaves and knits their conformability. Computational modelling is needed to achieve a goal of the IT Age, the virtual catwalk. The aim is to enable someone buying an article of clothing on-line to view on a screen how they would really look when moving around in the garment. There are three levels of reality in such simulations. In cartoons, unrealistic distortion is preferred. For realistic animation, in which film-makers have achieved great success, it is only necessary that the image should look right to the viewer. The third level, which is our concern, is to relate the fabric forms to the actual fabric properties and applied forces. This is much more difficult and some IT specialists who came optimistically to the problem have retreated. Leaving on one side the dynamic problem, the first step is to model the quasi-static buckling of textile fabrics in complex situations. Most researchers have attempted to solve the total problem by the use of finite-element or similar methods. However, such programs have not tackled the full anisotropy, which involves three in-plane and three out-of-plane modes of deformation, and the nonlinearity of textile fabrics. The models are limited in their validity, and are horrendously expensive in computer power and time.

A more fundamental approach is needed. Research should elucidate the basics of how fabrics buckle in three dimensions, and find clever ways, which are right for textile fabrics, to build up to the more difficult problems. Threefold buckling of an isotropic, Hookean circular specimen has been modelled by a central dome of double curvature and an outer zone of alternating folds of single curvature (Amirbayat, 1986). The sum of in-plane and out-of-plane strain energies and gravitational energy is minimized, using many simplifications. The approach needs to be improved and extended to remove mathematical infelicities and deal with multiple buckling of real fabrics, but it should show the way forward.

## CONCLUSION

At the operational level, the urgent need is for industrial application of the computational techniques developed for fabric structure and mechanics in the last 50 years – to match the advance of CAD for aesthetic design in the last 25 years. It is important that programs should be easy to use and provide the information that is needed in daily operations. Another Manchester development will help this. Many textile problems, notably the way of specifying a woven fabric structure, involve the selection of a small set of independent parameters from a large number of possible parameters that may be used. In order to avoid the need for separate programs for each independent set, *QAS* was programmed to run round a network of equations (Konopasek, 1970). This later led to the commercial program *TK Solver*. The network facility is included in *TechText CAD*.

At the academic level, the need is for research on treating the more difficult problems in clever ways, which are well adapted to the special features of fibre assemblies. Here the advance in computer power will help. In the 20<sup>th</sup> Century, we were constrained to treat problems in terms of small repetitive structural units or by statistical distributions of representative elements. In the 21<sup>st</sup> Century, there is the power to model the behaviour of large numbers of individual fibres or fibre elements. An example is the pioneering study of the compression of a random fibre assembly by Beil and Roberts at the University of Virginia. Other examples are carpet wear (Liu, 2003) and fabric pilling (Wilkins, 2004).