Mathematisches Forschungsinstitut Oberwolfach

Report No. 9/2005

Mini-Workshop: Mathematical Methods and Models of Continuum Biomechanics

Organised by
Ray W. Ogden (Glasgow)
Giuseppe Saccomandi (Lecce)

February 20th – February 26th, 2005

Abstract. The workshop *Mathematical Methods and Models of Continuum Biomechanics* focused on skills and tools providing a rational approach for integrating data that reductionist and molecular approaches in modern biological and medical science has recently provided. The workshop has provided contributions that brought together experts from the (bio-)mechanics and applied mathematics communities in order to highlight the mathematical needs and challenges especially in the fields of soft tissues and DNA mechanics.

Mathematics Subject Classification (2000): 74L15, 76Z05, 92C10, 92C35, 92D20.

Introduction by the Organisers

It is well known that biomechanics is rapidly becoming a classical field of application of mathematics. Several recently established societies and journals are devoted to this subject and increasingly many conferences are being organized with biomechanics as the central theme. However, continuum biomechanics remains to attract the attentions of significant numbers of mathematicians. Biomechanics has contributed much to understanding of human health and to disease and injury and their treatment, but has yet to reach its full potential as a consistent contributor to the improvement of health-care delivery. Because of the inherent complexities of the microstructure and biomechanical behaviour of biological cells and tissues, there is a need for new theoretical frameworks to guide the design and interpretation of new classes of experiments. Because of continued advances in experimental technology and the associated rapid increase in information on molecular and cellular contributions to the behaviour at tissue and organ levels, there is a pressing need for mathematical models to synthesize and predict observations across multiple length and time scales. And because of the complex geometries and loading conditions, there is a need for new computational approaches for the solution of

boundary- and initial-value problems of clinical, industrial and academic importance.

The investigations of particular interest in this framework are those that quantify the mechanical environment in which cells and matrix function in health, disease or injury, identify and quantify mechano-sensitive responses and their mechanisms, detail interrelations between the mechanical and biological processes such as growth, remodelling, adaptation and repair, and report discoveries that advance therapeutic and diagnostic procedures. For these investigations to be successful there is need for a strong mathematical background that differs from that in classical biomathematics.

First of all because, as noted in the 1998 Bioengineering Consortium (BECON) Report of the US National Institutes of Health,

The success of reductionist and molecular approaches in modern medical science has led to an explosion of information, but progress in integrating information has lagged. Mathematical models provide a rational approach for integrating this ocean of data, as well as providing deep insight into biological processes.

Second, because there are new challenges for such mathematical models that require review and revision of the axiomatic framework underpinning the usual analytical and computational models based on solid mechanics, fluid mechanics and thermo-mechanics, and their interactions. This means that there is a need to develop also new mathematical models.

The workshop *Mathematical Methods and Models of Continuum Biomechanics*, organized by Ray W. Ogden (Glasgow) and Giuseppe Saccomandi (Lecce) and held February 21st–26th, 2005, focused on this timely subject with contributions that brought together experts from the (bio-)mechanics and applied mathematics communities in order to highlight the mathematical needs and challenges in the field.

The topics addressed were:

mathematical modelling and computational issues in soft tissue mechanics with particular reference to growth and remodelling – this is a fundamental topic where there is the need for a new generation of mathematical tools for describing deformation as the mass and material properties change;

mathematical models and methods in cardiovascular systems – here the computational effort is striking, mainly for the study of blood flow in large arteries and in fluid-structure interaction problems; interesting mathematical problems come from associated multi-scale analysis and optimal control;

mathematical issues on the modelling of DNA - here the aim is to apply rigorous mathematical approaches and efficient computational algorithms in the development and application of models in order to understand the basic physical properties of DNA as a function of its base sequence; these properties are generally believed to be key to the biological function of DNA, but the mechanisms are not well understood.

The meeting was attended by 14 participants, a nice blend of researchers with various backgrounds. The program consisted of 14 talks and several informal discussions that benefited enormously from the unique academic atmosphere at the Oberwolfach Institute.

Mini-Workshop: Mathematical Methods and Models of Continuum Biomechanics

Table of Contents

Abstracts

Mathematical models of lipid membranes

Paolo Biscari

(joint work with Fulvio Bisi, Silvia Maria Canevese, Gaetano Napoli, Riccardo Rosso)

Lipid membranes are aggregates of amphiphilic molecules, which consist of a hydrophilic head and one or more hydrophobic tails. Living in an aqueous environment, these molecules tend to form bilayers where the hydrophobic parts are hidden by the hydrophilic ones, and so their contact with water is reduced. A further reduction is obtained when the bilayer closes itself to form a vesicle, which is modelled as a compact, two-dimensional surface.

We will first survey the classical results concerning the analysis of the elastic energy functional which determines the equilibrium vesicle shapes when both their area and enclosed volume are fixed [1, 2] . Proteins, thought of as rigid bodies, are usually modelled as small cones. When embedded in a lipid bilayer, they modify the membrane configuration by fixing the direction of the surface normal at the contact points [3].

In the two-dimensional approximation, where the membrane shape is modelled by a closed curve, we determine the exact equilibrium shape of the membrane in the presence of one or more proteins [4]. The excess of elastic energy induced by the proteins gives rise to a mediated interaction between them [5]. The interaction may be either attractive or repulsive, depending on the protein shape and relative distance [6, 7].

In the three-dimensional case, however, the panorama changes. The enclosed-volume constraint induces a double-infinity of stationarity shapes [8]. Moreover, a boundary layer analysis proves that the shape perturbations induced by the proteins are strongly localized and decay within a characteristic length-scale of the order of the protein diameter. Asymptotic methods allow to derive the analytical shape of the perturbation [9].

References

[1] W. Helfrich, *Elastic Properties of Lipid Bilayers: Theory and Possible Experiments*, Z. Naturforsch. C **28** (1973), 693–703.

[2] U. Seifert, K. Berndl, and R. Lipowsky, *Shape transformations of vesicles: Phase diagram for spontaneous-curvature and bilayer-coupling models*, Phys. Rev. A **44** (1991), 1182–1202.

[3] P. Helfrich and E. Jakobsson, *Calculation of deformation energies and configurations in lipid membranes containing gramicidin channels*, Biophys. J. (1990) **57**, 1057–1084.

[4] P. Biscari and R. Rosso, *Inclusions Embedded in Lipid Membranes*, J. Phys. A **34** (2001), 439–460.

[5] P. Biscari, F. Bisi, and R. Rosso, *Curvature Effects on Membrane-Mediated Interactions of Proteins*, J. Math. Biol. **45** (2002), 37–56.

[6] P. Biscari and F. Bisi, *Membrane-Mediated Interactions of Rod-like Inclusions*, Eur. Phys. Jnl. E **7** (2002), 381–386.

[7] P. Biscari, *Mediated Interactions of Proteins in Lipid Membranes*. In "Rational Continua, Classical and New", ed. Springer (2003), 11-18.
[8] P. Biscari, S.M. Canevese, and G. Napoli, *Impermeability effects in three-dimensional vesicles*, J. Phys. A **37** (2004), 6859–6874.
[9] P. Biscari and G. Napoli, *Nonlinear shape perturbations induced by vesicle inclusions*, to appear (2005).

Flaw tolerant nanoscale and hierarchical structures of biological materials

Huajian Gao

One of the most exciting challenges to materials science in the 21st century is the development of multi-functional and hierarchical materials systems. Nanotechnology promises to enable mankind to eventually design materials using a bottom-up approach by tailor-designing microstructures from atomic scale and up. Before these objectives can be realized, some important questions need to be addressed. How can a hierarchical material be designed in a systematic way to achieve a particular set of properties? How to bridge different levels of structural hierarchy? What is the criterion to choose the characteristic length scales for all hierarchical levels? What is the theoretical basis for bottom-up design of materials? Motivated by the above questions, we have performed a series of studies (see papers cited below and references therein) of the mechanical properties of the nanostructures of hard biological tissues like bone and shells. These studies have led to a concept called flaw tolerance which is defined as a state of material in which pre-existing cracks do not propagate even as the material is stretched to failure near its limiting strength. In this process, the material around the crack fails not by crack propagation, but by uniform rupture at the limiting strength. This concept provides a nice analogy between known concepts and phenomena in fracture mechanics and robust designs of nanoscale and hierarchical structures of biological materials. Biological materials are known to have complex hierarchical structures over many length scales. While sea shells exhibit 2 to 3 levels of lamellar structure, bone has been categorized into having 7 levels of hierarchy. Although the higher levels of structural hierarchy show great complexity and variations in different biological materials, it is interesting to observe that nature exhibits a convergent evolution at the nanostructure level in that the smallest building blocks of biological materials are generally designed at the nanoscale with nanometer sized hard inclusions embedded in a soft protein matrix. In tooth enamel, this nanostructure consists of needle-like (15-20nm thick and 1000nm long) crystals embedded in a relatively small volume fraction of a soft protein matrix. In dentin and bone, the corresponding nanostructure consists of plate-like (2-4 nm thick and up to 100 nm long) crystals embedded in a collagen-rich protein matrix, with the volume ratio of mineral to matrix on the order of 1:2. The elementary structure of nacre is made of plate-like crystals (200-500 nm thick and a few micrometers long) with a very small amount of soft matrix in between. All of the biological nanostructures share

the common feature of hard inclusions with a very large aspect ratio arranged in a parallel staggered pattern in a soft matrix. Similar design principles have also been used in the cell walls of wood made of hard cellulose fibrils embedded in a soft hemicellulose-lignin matrix. In the past, numerous studies have been carried out to understand the high toughness of biological materials from various points of view. Recent investigations in our research group have also addressed the questions of why the elementary structure of biocomposites is designed at the nanometer length scale and how the toughness and other mechanical properties are related to the nanostructure. However, up to now there is still a lack of understanding of the general design principles for the structural hierarchy of biological materials. As a first step toward understanding the basic design principles of nature, we note that biological materials like bone must be able to survive crack-like flaws of many size scales in order to successfully perform their designated mechanical and biological functions. The self-sensing, self-adapting and self-repairing capabilities of bone require not only a dynamical network of blood vessels for supply of nutrient, but also constant removal and replacement of old and damaged materials with fresh and healthy materials. The fact that all these processes should occur at the same time while an animal is conducting its normal activities indicates that biological materials must be designed to tolerate crack-like flaws of many size scales. We have found it useful to adopt the concept of flaw tolerance as a basic principle in understanding the nanostructure of biological systems. On the one hand, the concept of flaw tolerance can be related to the concepts of notch insensitivity, fracture size effects and large scale yielding or bridging in fracture mechanics; on the other hand, it can also be related to the theory of evolution which states that survivability (in this case against mechanical flaws) is a key to propagation of animal species. In this way, the concept of flaw tolerance provides an important analogy between the known concepts and phenomena in fracture mechanics and new effort on failure mechanisms of nanostructures and biological systems. In the state of flaw tolerance, pre-existing crack-like flaws do not propagate and do not participate in the failure process. This view has formed a central theme in our recent studies on the protein-mineral nanostructure of bone as well as the mechanics of hierarchical adhesion systems of gecko. In various biological systems, it has been shown that, as the characteristic size of the critical structural link is reduced to below a critical size, a class of elastic solutions emerge with the interesting feature of uniform stress distribution even in the vicinity of a crack. The idea of flaw tolerance has been used to explain the nanometer sizes of mineral crystals in bone and of the adhesive nanoprotrusions of gecko. In a flaw tolerant biological system, failure occurs not by propagation of a pre-existing crack, but by uniform rupture at the limiting strength of the material. The concept of flaw tolerance emphasizes the intrinsic capability of a material to tolerate crack-like flaws of all sizes. Since the crack size and geometry is not explicitly considered, this concept is particularly useful in the study of hierarchical materials where a mixing of flaw geometry with multiple characteristic sizes of the structural hierarchies would greatly complicate the problem. A dimensionless number, called the flaw tolerance number

in analogy with the Reynolds number in fluid mechanics, has been introduced to characterize the transition from Griffith fracture to flaw tolerance state as the size of material is reduced to below a critical length scale. It has been estimated that the critical length for flaw tolerance can vary from near atomic scale for materials like diamond with high Young's modulus and more perfect atomic structures to a few hundred nanometers for biominerals which have relatively low Young's modulus with less perfect lattice structure and less pure chemical constituents. Flaw tolerance corresponds to optimizing strength taken into consideration of potential crack-like flaws. For homogeneous materials, there is always a critical length scale which is usually on the order of nanometer length scales for brittle materials and on the order of micrometer length scales for ductile materials like metals. Is it possible to design materials that can tolerate crack-like flaws at macroscopic scales without size limit? Can we design materials of any macroscopic size which still remains capable of tolerating all internal crack-like flaws? To answer these questions in a qualitative way, we have made use of the concept of flaw tolerance to demonstrate the enormous potential of hierarchical material design by considering a hierarchical material with self-similar structures mimicking the nanostructure of bone. This "fractal bone" exhibits a similar microstructure at all hierarchical levels consisting of a staggered hard phase embedded in a soft matrix; the hard phase provides the structural rigidity while the soft phase absorbs and dissipates fracture energy. Simplified analytical models are adopted to evaluate the stiffness, strength and fracture energy at each level of structural hierarchy based on properties from the substructure one level below. The characteristic size of the hard phase at each hierarchical level is determined based on the principle of flaw. It is shown that this bottom-up designed material can tolerate crack-like flaws of all sizes, from nanoscale up to macroscopic scales with no size limit.

References

[1] Gao, H., Ji, B., Jaeger, I.L., Arzt, E., Fratzl. P. *Materials become insensitive to flaws at nanoscale: lessons from nature*, Proc. Natl. Acad. Sci. USA **100** (2003), 5597-5600.

[2] Gao, H., Ji, B., *Modeling fracture in nanomaterials via a virtual internal bond method*, Eng. Frac. Mech. **70** (2003), 1777-1791.

[3] Gao, H., Ji, B., Buehler, M. J., Yao, H. *Flaw tolerant bulk and surface nanostructures of biological systems*, Mech. Chem. Biosys. **1** (2004), 37-52.

[4] Gao, H., Yao, H. *Shape insensitive optimal adhesion of nanoscale fibrillar structures*, Proc. Natl. Acad. Sci. USA **101** (2004), 7851-7856.

[5] Gao, H., Wang, X., Yao, H., Gorb, S., Arzt, E. *Mechanics of hierarchical adhesion structure of gecko* , Mech. Mat. **37** (2005), 275-285.

[6] Gao, H., Chen, S. *Flaw tolerance in a thin strip under tension* , J. Appl. Mech., in the press.

[7] Ji, B., Gao, H. *Mechanical properties of nanostructure of biological materials*, J. Mech. Phys. Solids **52** (2004), 1963-1990.

[8] Ji, B., Gao, H. *A study of fracture mechanisms in biological nano-composites via the virtual internal bond model* , Mater. Sci. Eng. A **366** (2004), 96-103.

[9] Ji, B., Gao, H. *Flow stress of biomorphous metal-matrix composites*, Mater. Sci. Eng. A **386** (2004), 435-441.

[10] Ji, B., Gao, H., Hsia, K.J. *How do slender mineral crystals resist buckling in biological materials?* Phil. Mag. Lett. **84** (2004), 631-641.

Elastic growth and instability in soft tissues

Alain Goriely
(joint work with Martine Ben Amar)

Growth in elastic materials can produce stress either through incompatibility of growth or by interaction with the surrounding medium. The central question addressed by the authors is whether the stress induced through growth is sufficient to induce shape instability in the growing medium. Related questions are whether growth plays a role in physiological conditions to help stabilize and regulated mechanical loads and how macroscopic properties of tissues and plants are inherited through the growth process.

At the biomechanical level, soft-tissues with possibly large strains and nonlinear anisotropic behavior are best represented by hyperelastic materials and modeled within the theory of finite elasticity in which their response to stress is determined by a strain energy function [1]. The modeling of such functions for tissues with given symmetries represents an important and active field of study [2, 3]. Growth can be modeled by a multiplicative decomposition of the deformation gradient due to Rodriguez *et. al.* [4] similar to the one found in elasto-plasticity [5]. The deformation tensor is assumed to be a product of a growth tensor describing the local evolution of a mass element with no geometric or external constraint and an elastic response of the material describing the strain necessary to ensure integrity and compatibility of the material. This theory of material growth and its various generalizations have been applied successfully to the modeling of many physiological systems such as arteries, cartilage, muscle fibers, heart tissues and solid tumors [1]. The growth tensor can be coupled to the strain and stress fields, the material position in the medium, the density of nutrients, or the concentration of morphogens. Of particular interest for the present study, is the problem of differential growth where growth depends on the position inside the tissue. Differential growth is known to be of fundamental importance in development where it is responsible for shape formation [6].

To gain better insight in growth-induced instabilities, the growth of an elastic shell loaded with hydrostatic pressure or embedded in an elastic medium has been studied. Three cases have been considered: *(i)* a constant but anisotropic growth respecting the spherical symmetry, *(ii)*, the radially differential growth of a shrinking sphere and *(iii)* the case of a growing shell embedded in an elastic medium. The residual stress arising from the incompatibility of growth and the contact stress arising from the interaction with the surrounding medium are computed with respect to growth and geometric parameters and critical values for instability are obtained. Depending on these parameters, different modes of instability can be obtained. These results have been presented in two articles by the authors [7]

References

[1] J. D. Humphrey. Continuum biomechanics of soft biological tissues. *Proc. Roy. Soc. Lond. A*, 459:3–46, 2003. S. C. Cowin. Tissue growth and remodeling. *Annu. Rev. Biomed. Eng.*,

6:77–107, 2004. S. M. Klisch, S. S. Chen, R. S. Sah and A. Hoger. A Growth Mixture Theory for Cartilage With Application to Growth-Related Experiments on Cartilage Explants. *J. Biomech. Engineering*, 125:169–179, 2003.

[2] Y. C. Fung. *Biomechanics: material properties of living tissues*. Springer, New York, 1993.

[3] G. A. Holzapfel, T. C. Gasser, and R. W. Ogden. A new constitutive framework for arterial wall mechanics and a comparative study of material models. *J. Elasticity*, 61:1–48, 2000.

[4] E. K. Rodriguez, A. Hoger, and McCulloch A. Stress-dependent finite growth in soft elastic tissue. *J. Biomechanics*, 27:455–467, 1994.

[5] E. H. Lee. Elastic-plastic deformation at finite strains. *J. Appl. Mech.*, 36:1–8, 1969.

[6] U. Kutschera. Tissue stresses in growing plant organs. *Physiologia Plantarum*, 77:157–163, 1989. J. Dumais, C. R. Steele and S. C. Rennich. New evidence for the role of mechanical forces in the shoot of apical meristem. *J. Plant Growth Regul.*, 19:7–18, 2000. P. D. Shipman and A. Newell. Phyllotactic patterns on plants. *Phys. Rev. Lett.*, 92: 168102, 2004.

[7] M. Ben Amar and A. Goriely, *Growth and instability of soft tissues*, Preprint (2004). A. Goriely and M. Ben Amar *Differential growth and instability in elastic shells*, Preprint (2005)

Pulmonary airway closure – a large-displacement fluid-structure interaction problem

Matthias Heil

(joint work with Andrew Hazel and Joseph P. White)

The gas-conducting airways of the lung are flexible tubes lined with a thin liquid film. The film is susceptible to a capillary instability, analogous to the classical Plateau–Rayleigh instability, provided that the length of the airway is greater than the circumference of the air-liquid interface. The instability causes an initially-uniform film to develop a series of axisymmetric peaks and troughs. The fluid pressure is low in the regions of increased film height, the lobes, and the compressive load on the airway walls is locally elevated in these regions.

We develop an idealised model of the liquid-lined pulmonary airways and study their behaviour using a fully-coupled, three-dimensional finite-element method. The deformations of the airway wall are modelled using Kirchhoff–Love, thin-shell theory and the dynamics of the liquid film are described by the Navier–Stokes equations.

Our simulations to show that, if the surface tension of the liquid is sufficiently high, relative to the bending stiffness of the tube, the altered loading induced by the primary axisymmetric instability can lead to a secondary, non-axisymmetric, buckling instability of the elastic airway wall. Under certain conditions, the subsequent evolution of the system leads to complete occlusion of the gas core by the liquid — airway closure. Furthermore, we demonstrate that non-axisymmetric instabilities allow the occurrence of airway closure at fluid volumes that are too small to form occluding liquid bridges in an axisymmetric geometry. A typical example of our simulations is shown in Figure 1.

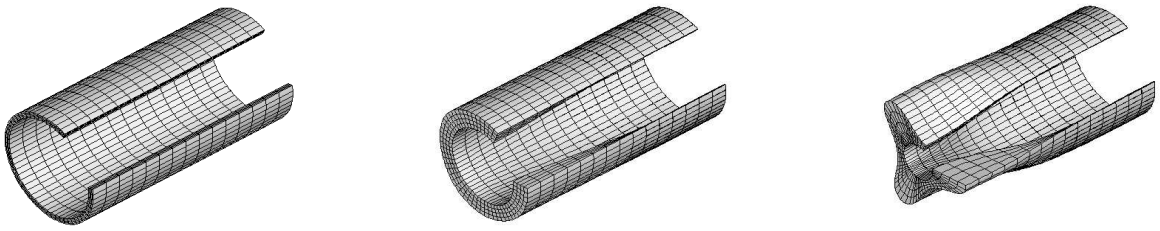

FIGURE 1. An initially-uniform liquid film undergoes an axisymmetric capillary instability causing fluid to drain into a lobe. The additional compressive load in the region of the lobe causes the elastic tube to buckle non-axisymmetrically and, ultimately leads to airway closure. Time increases from left to right and the liquid is shown as a shaded volume. In the simulation, symmetry conditions are imposed at both ends of the tube and hence only one half of the developing lobe is shown.

Constitutive restriction on swelling

JACQUES MARIE HUYGHE

Swelling of saturated porous media is associated either with affinity between the porous solid and the fluid or with ionisation of the porous solid compensated by an opposite ionisation of the fluid. Constitutive restriction are formulated for an elastic ionised porous solid saturated with an aqueous solution of a monovalent salt and subject to finite deformation. Unlike other authors dealing with saturated porous media [2, 3, 5, 4] equipresence is strictly adhered to. The full constitutive description is contained in (1) a free energy of the mixture and (2) a frictional matrix. The independent constitutive variables are the Green strain, the Lagrangian velocities of the fluid, cations and anions relative to the solid, and the composition of the mixture. The entropy inequality requires that the free energy of the mixture does not depend on the relative velocities. This is a very important result that is true for elastic saturated porous media in general, and was missed by [2, 3]. Instead, Bowen *assumes* the partial free energies not to depend on relative velocities, without justification. From our analysis, it appears that the total free energy , the total stress of the mixture and the electrochemical potentials of the fluid, cations and anions cannot be dependent from the relative velocities, which is consistent with an assumption of Biot [1]. The reason why the result was missed by other mixture theorists is that they used an Eulerian description for solid, while we are using a Lagrangian description. We do not see any arguments to assume the *partial* free energies are independent from the relative velocities as assumed by Bowen [3] in eq. 3.1. The chemical expansion stress used by other swelling theories [4] is not

consistent with the constitutive restrictions derived by us. The electrostatic interactions between the charges are included through an electroneutrality condition. Unlike Lai et al. [4], we introduce the electroneutrality condition into the entropy inequality through a Lagrange multiplier which is physically interpreted as an electrical potential [6, 8]. Streaming and diffusion potentials, streaming and diffusion currents, electro-osmosis, electrophoresis, chemical osmosis, Donnan osmosis, Donnan exclusion and Donnan potentials are some of the physical phenomena typically described. The model is experimentally validated for intervertebral disc tissue [7] as well as for hydrogel [9]. It is implemented into a 3D finite deformation FE model by van Loon et al. [11] and finds applications in wellbore stability [10], bone remodelling [12], skin research [13] and cellular physiology [14].

References

[1] M. Biot, *Theory of finite deformation of porous solids* Indiana University Math.J. **21** (1972), 597–620.

[2] R.M. Bowen, *Incompressible porous media models by the use of the theory of mixtures*, Int. J. Eng. Sci. **18** (1980), 1129–1148.

[3] R.M. Bowen, *Compressible porous media models by the use of the theory of mixtures*, Int. J. Eng. Sci. **18** (1982), 697–735.

[4] W.M. Lai, J.S. Hou and V.C. Mow, *A triphasic theory for the swelling and deformation behaviours of articular cartilage*, J. Biomech.Eng. **113** (1991), 245–258.

[5] S. Achanta, J. Cushman, and M. Okos . *On multicomponent, multiphase thermodynamics with interfaces*, Int. J. Eng. Sci. **32** (1994), 171–1738.

[6] J.M. Huyghe and J.D. Janssen *Quadriphasic theory of swelling incompressible porous media*, Int. J. Engng. Sci. **35** (1997), 793–802.

[7] A.J.H. Frijns , J.M. Huyghe and J.D. Janssen, *A validation of the quadriphasic mixture theory for intervertebral disc tissue*, Int. J. Engng. Sci., **35** (1997). 1419-1429.

[8] J.M. Huyghe and J.D. Janssen *Thermo-chemo-electro-mechanical formulation of saturated charged porous solid*, Transp. Porous Media. **34** (1999), 129–141.

[9] A.J.H. Frijns , J.M. Huyghe, E.F. Kaasschieter and J.D. Janssen, *Numerical simulation of deformations and electrical potentials in a cartilage substitute*, Biorheology, **40** (2003). 123-131.

[10] M.M. Molenaar and J.M. Huyghe, *An electro-chemo-mechanical mixture formulation of shale* in 'Chemo-mechanical coupling in clays' ed. by C. Di Maio, T. Hueckel and B. Loret , Swets and Zeitlinger, Lisse, The Netherlands (2002), 247–260.

[11] R. van Loon, J.M. Huyghe, M.W. Wijlaars and J.D. Janssen *3D FE implementation of an incompressible quadriphasic mixture model*, Int. J. Num. Meth. Engng. **57** (2003), 1243–1258.

[12] J.M. Huyghe and T. Smit *Comment les cellules de l'os ressentent-elles une contrainte mécanique?*, Arch. Physiol. Biochem. **112** (2004), 48–50.

[13] P.M. van Kemenade, M.M.J Houben, J.M. Huyghe and L.F.A. Douven *Do osmotic forces play a role in the uptake of water by human skin*, Skin Res. Technol. **10** (2004), 109–112.

[14] C.C. Donkelaar, M.A. Daniels, J.M. Huyghe,*Cell deformation in response to long term hyperosmotic loading* Acta Bioeng. Biomech. **5** (2003), 1–10.

Modelling and simulation of biological growth phenomena

Ellen Kuhl

(joint work with Grieta Himpel, Andreas Menzel, Paul Steinmann)

This contribution aims at discussing different strategies to model and simulate growth phenomena typically encountered in hard and soft tissues. Roughly speaking, existing models for growth, or rather changes in mass, can be classified in two basic categories: models based on changes in density and models based on changes in volume. While the former are typically characterized through a mere constitutive coupling between growth and deformation, the latter rather introduce a kinematic coupling.

The first class of models dates back to the early work of Cowin and Hegedus [1] and is sometimes referred to as theory of adaptive elasticity. Based on the thermodynamics of open systems, it was primarily designed for density growth at constant volume characteristic for open pored hard tissues such as bones, see also [4].

The second class of models was pioneered by Rodriguez, Hoger and Mc Culloch [7]. Motivated by the development of multiplicative plasticity, they introduce an incompatible growth configuration and perform a multiplicative decomposition of the deformation gradient into a growth part and an elastic part. Models of this second class, which nicely capture volume growth at constant density, are predominantly designed for growth in soft tissues, see [3], [2].

In addition to changes in mass, we also address the aspect of remodelling, i.e. the reorientation of fibers in anisotropic biological tissues as illustrated in [5, 6].

We present a systematic comparison of the individual approaches and illustrate how the different strategies can be combined in a single unique framework. Numerical examples illustrate the basic features of density growth, volume growth and fiber reorientation in the context of hard and soft tissue mechanics.

References

[1] S. C. Cowin and D. H. Hegedus, *Bone remodelling I: Theory of adaptive elasticity*, J. Elasticity, Vol. 6, pp. 313–326, (1976)

[2] G. Himpel, E. Kuhl, A. Menzel and P. Steinmann,, *Computational modelling of isotropic multiplicative growth*, Comp. Mod. Eng. Sci., accepted for publication.

[3] V. A. Lubarda and A. Hoger, *On the mechanics of solids with a growing mass*, Int. J. Solids & Structures, Vol. 39, pp. 4627–4664, (2002)

[4] E. Kuhl, A. Menzel, and P. Steinmann, *Computational modeling of growth: A critical review, a classification of concepts and two new consistent approaches*, Comp. Mech., Vol. 32, pp. 71–88, (2003)

[5] E. Kuhl, A. Menzel, and K. Garikipati, *On the convexity of transversely isotropic chain network models*, Phil. Mag., accepted for publication.

[6] E. Kuhl, K. Garikipati, E. M. Arruda and K. Grosh, *Remodeling of biological tissue: Mechanically induced reorientation of a transversely isotropic chain network*, J. Mech. Phys. Solids, http://arxiv.org/abs/q-bio.QM/0411037, accepted for publication.

[7] E. K. Rodriguez, A. Hoger and A. D. Mc Culloch, *Stress–dependent finite growth in soft elastic tissues*, J. Biomechanics, Vol. 27, pp. 455–467, (1994)

Helices

John H. Maddocks
(joint work with N. Choaïeb, A. Goriely)

It is shown that a uniform and hyperelastic, but otherwise arbitrary, non-linear Cosserat rod has helices as the centerline of equilibrium configurations. For anisotropic rods, and for each of the local two-parameter family of helical centerlines corresponding to changes in the radius and pitch, there are a discrete number, greater than or equal to two, of possible orientations of the cross-section at equilibrium. The possible orientations are characterized by a pair of finite-dimensional, dual variational principle involving point-wise values of the strain-energy density and its conjugate function. For sufficiently short helical segments, members of the two parameter family in this variational principle are stable in the sense that they are local minima of the total elastic energy for the corresponding boundary value problem. This theoretical problem has practical applications in different fields such has structural mechanics, civile engineering, biochemistry and biology. Detailed discussion of the implication of such problem in the study of the supercoiled structure of DNA is provided.

References

[1] N. Choaïeb, J. H. Maddocks , *Kirchhoff's Problem of Helical Equilibria of Uniform Rods*, J. of Elasticity, to appear (2005).
[2] N. Choaïeb, A. Goriely, J. Maddocks , *Helices*, in preparation (2005).

Why a Mixed Hybrid Formulation for Four-Component Modelling of Cartilaginous Tissues?

Kamyar Malakpoor
(joint work with E.F. Kaasschieter, J.M.R. Huyghe)

Swelling and shrinking behavior of cartilaginous tissues (like intervertebral disk) can be modelled by a four-component mixture theory in which a deformable and charged porous medium is saturated with a fluid with dissolved ions [1]. This theory results in a coupled system of non-linear parabolic partial differential equations together with an algebraic constraint for electro-neutrality.

There are two major phases of cartilaginous tissue. A fluid phase containing liquid and electrolytes (cations and anions) and a solid phase containing collagen fibers and protoeglycans. The tissue can shrink only by expelling water and can swell only by attracting water. Mixture theory can be used to model of these phenomena in the framework of thermodynamics. The linear elastic solid matrix and the fluid are assumed to be intrinsically incompressible.

For the sake of local mass conservation a mixed variational formulation seems to be a good choice for the numerical algorithm. The solid displacement, fluid flow, ion fluxes and electro-chemical potentials are chosen to be the primitive variables.

One of the requirements for the stability of the method is that the divergences of the fluxes must be in L^2. In fact, this condition states that the normal components of fluxes are continuous across the inter-element boundaries. In our model this condition is not satisfied for the ion fluxes. The reason is that the ion fluxes may have jumps over inter-element boundaries and therefore cannot have the required regularity. To prevent this problem we consider hybridization of the mixed formulation. This will introduce Lagrange multipliers to relax the continuity requirement for the fluxes across the internal edges.

References

[1] J.M.R.J. Huyghe, J.D. Janssen, *Quadriphasic mechanics of swelling incompressible porous media*, Int. J. Engng Sci., 35, 793-802, (1997).

Fibre reorientation for transversely isotropic and orthotropic tissue adaptation

Andreas Menzel

(joint work with Ellen Kuhl)

Biological tissues posses various sub-structures on different length scales. Consequently, the macroscopic behaviour of these materials is highly anisotropic. The self-organisation of biological tissues or rather deformation induced evolution of representative underlying sub-structures are of cardinal interest for the modelling of, e.g., hip implants, wound healing, balloon angioplasty, tissue engineering, etc. To give an example, connective tissue is criss-crossed by collagen which bears most of the applied stress. These collagen fibres adapt with respect to the dominant loading directions.

From a macroscopic point of view the framework of fibre reinforced materials allows combination with isotropic growth theories based on open system mechanics. The proposed phenomenological model is based on the introduction of structural tensors as key (internal) variables. Apparently, these fields conveniently enable the description of anisotropic response. For a review on theoretical and numerical issues on the evolution of structural tensors embedded into a general framework for finite inelasticity see [6]. Based on these additional structural arguments, anisotropic remodelling is addressed via appropriate evolution equations for the underlying fibre directions and diameters while volumetric remodelling is realized by the evolution of the density field. The fibre direction evolution might either be based on an alignment with respect to appropriate stress fields, as for instance applied in [1, 2], or according to suitable deformation tensors. The latter approach has been developed within an open system continuum growth theory in [4, 5] and is also adopted for an anisotropic chain model in [3]. The advocated theoretical reorientation framework is mainly motivated by the contributions [8, 7]. Conceptually speaking, the structural tensors evolve in a (viscous) time dependent

manner so that stress and strain fields finally commute. This property renders the strain energy to be a critical point at a given deformation tensor. Unlike classical engineering materials, however, living bio-materials tend to strengthen rather than degrade in response to loading. Accordingly, at its critical value, the strain energy can either take a local minimum as in traditional mechanics or even a local maximum.

Until now, reorientation models have been developed for transversely isotropic materials based on one single fibre family. In this contribution, the approach advocated in [4] has been extended to orthotropic response. Two mechanically different fibre families are incorporated and assumed to remain orthogonal during the entire deformation process. Consequently, both vector fields follow one and the same proper orthogonal reorientation. The computation of this transformation is performed in four steps:

(i) construction of a rotation tensor in terms of the principal strain directions and an orthonormal frame with respect to the fibre families
(ii) computation of the corresponding rotation angle and axis
(iii) scaling of the (pseudo) rotation vector which serves as an ansatz for the angular velocity vector of both fibre families
(iv) integration over time and computation of the actual fibre orientations

The developed algorithm nicely fits into standard numerical tools like for instance nonlinear finite element codes. Several (open) problems might constitute related future research:

(a) elaboration of different reorientation models which, in the present context, addresses different arrangements of the orthonormal frames in (i)
(b) coupling with residual/initial stresses and/or strains
(c) stability analysis
(d) elaborations on critical points of the strain energy where principal strain directions do not coincide with the two fibre families
(e) elaborations on universal relations for orthotropic materials
(f) elaborations on the time scale of adaptation
(g) comparison with experiments

References

[1] S. Imatani and G.A. Maugin, *A constitutive model for material growth and its application to three-dimensional finite element analysis*, Mech. Res. Comm. **29** (2002), 477–483.
[2] G. Johansson, A. Menzel, and K. Runesson, *Modeling of anisotropic inelasticity in pearlitic steel at large strains due to deformation induced substructure evolution*, (2005) submitted for publication.
[3] E. Kuhl, A. Menzel, and K. Garikipati, *On the convexity of transversely isotropic chain network models*, Phil. Mag. (2005) accepted for publication.

[4] A. Menzel, *Modelling of anisotropic growth in biological tissues – a new approach and computational aspects*, Biomech. Model. Mechanobio. (2005) DOI:10.1007/s10237-004-0047-6, in press.
[5] A. Menzel, *Anisotropic remodelling of biological tissues*, In G.A. Holzapfel and R.W. Ogden, editors, IUTAM Symposium on Mechanics of Biological Tissue (2005) Springer, accepted for publication.
[6] A. Menzel and P. Steinmann, *On the spatial formulation of anisotropic multiplicative elasto–plasticity*, Comput. Methods Appl. Mech. Engrg. **192** (2003) 3431–3470.
[7] C. Sgarra and M. Vianello. *Rotations which make strain and stress coaxial*, J. Elasticity **47** (1997) 217–224.
[8] M. Vianello. *Optimization of the stored energy and coaxiality of strain and stress in finite elasticity*, J. Elasticity **44** (1996) 193–202.

Twisted rod theory applied to the supercoling of DNA

Sébastien Neukirch

We use an elastic rod model with contact to study the extension versus rotation diagrams of single supercoiled DNA molecules. We reproduce quantitatively the supercoiling response of overtwisted DNA and, using experimental data, we obtain an estimate of the effective supercoiling radius and of the twist rigidity of B-DNA. We find that the twist rigidity of DNA seems to vary widely with the nature and concentration of the salt buffer in which it is immersed.

Primarily the DNA molecule simply is the carrier of our genetic code. But in order to understand how a 2 m long string of DNA can fit into a 10 μm nucleus, one has to also consider its mechanical properties, namely the fact that the DNA double helix is a long and thin elastic filament that can wrap around itself or other structures. These mechanical properties will in general depend on the sequence of base pairs (bp) of which the molecule is made. Nevertheless the behavior of long molecules, i.e. more than a hundred bp, is well described by coarse-grained models such as twisted rods elasticity.

In the magnetic tweezer experiment [1] a single DNA molecule is anchored on a glass surface at one end, and glued to a magnetic bead at the other end. The molecule is pulled and twisted with the help of a magnet that acts on the bead. Experiments are carried under constant force. The end-to-end distance z of the DNA molecule, which is measured thanks to a microscope, is recorded together with the number of turns, n, made on the bead. Then under gradually increased rotation, the extension z decreases with the number of turns, n, put in and eventually the molecule starts to wrap around itself. Geometrically speaking, the DNA molecule is coiling around itself in a helical way. Since the molecule is already a double helix, we refer to this as supercoiling. Each helical wave of the super helix is called a plectoneme.

We present an elastic model that includes self-contact but leaves out thermal fluctuations. Our point is that, in the regime where plectonemes are formed, the relevant physical information is already present in our zero-temperature elastic rod

model with hard-wall contact. The model enables us to extract from experimental data the supercoiling radius as well as the ratio of the bending rigidity to the twist rigidity of the molecule.

References

[1] T. R. Strick, J.-F. Allemand, D. Bensimon, A. Bensimon, and V. Croquette. The elasticity of a single supercoiled DNA molecule, *Science*, **271** (1996) 1835–1837

Arterial tissue mechanics and stress-induced growth

Ray Ogden
(joint work with Anna Guillou)

In this talk we first outlined the structural properties of arterial wall tissue, with particular reference to the collagen fibre constituents that endow the material with a strongly anisotropic character. Relevant stress-strain experimental data that illustrate the nonlinearly elastic response of the material were also highlighted along with the important role of residual stress. Background and detailed references can be found in [1, 2]. The equations of nonlinear elasticity that form the basis for constructing material models were then discussed and results for a particular choice of constitutive law applied to extension and inflation of a thick-walled circular cylindrical tube were obtained to illustrate the predictions of the model. Particular reference to the influence of residual stress on the stress distribution through the tube wall at normal physiological pressures was a feature of the work. A method of taking the distribution of collagen fibre directions into account on the basis of a 'generalized structure tensor' was also discussed briefly.

In the second half of the talk, based on the recent work by Guillou and Ogden [3], we introduced a general theory of growth that takes account of the interaction between growth (changing mass) in soft tissue and mechanical stress. For this purpose the modifications of the usual mass and momentum balance equations of continuum mechanics required to accommodate changing mass were highlighted. A new form of constitutive law based on a free energy that depends on density, density gradient, the total deformation gradient (relative to a fixed reference configuration), structure tensors and residual stress was then discussed along with a general form of growth law.

A general elastic/growth boundary-value problem was then formulated, which, in principle, allows both the changing density and the deformation to be calculated for any given form on constitutive law for the stress and growth. It also enables the residual stress (and the evolving unloaded configuration) associated with the growth to be determined. The theory was then applied to an artery wall under hypertensive stress in order to illustrate the change in wall thickness due to growth using a very simple example.

References

[1] G. A. Holzapfel, T. C. Gasser, R. W. Ogden, *A new constitutive framework for arterial wall mechanics and a comparative study of material models*, Journal of Elasticity **61** (2000), 1–48.

[2] G. A. Holzapfel, R. W. Ogden, *Biomechanics of Soft Tissue in Cardiovascular Systems*, CISM Courses and Lectures Series **441**, Springer, Wien (2003).

[3] A. Guillou, R. W. Ogden, *Growth in Soft Biological Tissue and Residual Stress Development*, Proceedings of the IUTAM Symposium on Mechanics of Biological Tissue, Graz, Austria, June 2004, in press.

Recent insights in the mathematics and mechanics of rubber-like and biological materials

Giuseppe Saccomandi

The aim of the present talk is to show that some of the techniques and methods that have been developed to model the mechanical behavior of natural rubber and elastomers may be used successfully to understand biological materials. For example, rubber-like materials and a large class of biological materials exhibit a significant stiffening or hardening in their stress-strain curves at large strains. Considerable progress has been made recently in the phenomenological modelling of this effect within the context of isotropic and anisotropic hyperelasticity. In particular, constitutive models reflecting limiting chain extensibility may be successful used to generalize in a $3-D$ setting one dimensional molecular models as the freely jointed chain and the worm-like-chain. These phenomenological models may be generated on using a modification of a systematic scheme proposed by Rivlin and Signorini. This generalization is obtained by considering an approximation based on rational functions instead polynomials. This more general setting allows to have a control on the various constitutive parameters introduced to avoid difficulties that may be arise in the fitting of experimental data. Moreover, we show that this approach is successful not only to describe data in simple tension experiments, but also to describe more complex effects as Mullin's effect and this on the basis of the mechanism of network alteration. Network alteration is fundamental to study the ageing of biological tissues. In such a way it is possible to have a more deep understanding of the constitutive issues related to the mathematical modelling to the mechanical properties of biological materials at both the microscopic scale (in the case of proteins such as elastin, collagen or DNA) and the macroscopic scale (in the case of tissues such as arterial walls).

The present research is supported by the PRIN2004 project *Modelli Matematici per la Dinamica del DNA*.

References

[1] C. O. Horgan, G. Saccomandi, *Constitutive modelling of rubber-like materials and biological materials with limiting chain extensibility*, Mathematics and Mechanics of Solids **7** saccomandi1(2002) 353–371.

[2] E. Pucci, G. Saccomandi, *A note on the Gent Model for rubber-like materials*, Rubber Chemistry and Technology **75** (2002) 839–851.
[3] C. O. Horgan, G. Saccomandi, *A molecular-statistical basis for the Gent model of rubber elasticity* J. of Elasticity, **68** (2002) 167–176.
[4] C. O. Horgan, G. Saccomandi, *Finite thermoelasticity with limiting chain extensibility*, Journal of Mechanics and Physics of Solids **75** (2003) 839–851.
[5] C. O. Horgan, G. Saccomandi, *A description of arterial wall mechanics using limiting chain extensibilty constitutive models* Biomechanics and Modeling in Mechanobiology **1** (2003) 251–266.
[6] C. O. Horgan, R. W. Ogden, G. Saccomandi, *A theory of stress softening of elastomers based on finite chain extensibility* Proceedings Royal Society of London A **460** (2004) 1737–1754.
[7] R. W. Ogden, G. Saccomandi, I. Sgura, *Fitting hyperelastic models to experimental data* Computational Mechanics **34** (2004) 484–502.

Numerical studies of nonlinear lattice models for DNA dynamics

Ivonne Sgura
(joint work with Giuseppe Saccomandi)

In the process of DNA replication, transient opening of base pairs and its propagation can be modelled as a solitary wave moving along the strands. To give motion equations when a strand is represented as a lattice of N particles, the analogy with a mechanical system that allows soliton solutions has been proposed by many authors (see e.g. [7]).

In this talk we focus on some special solitons with compact support, called compactons, whose existence has been proved in nonlinear dispersive PDEs [5, 6]. The non smooth interface of compactons and nonlinearities of the equations present significant theoretical and numerical challenges. In fact, compactons are usually weak solutions of PDEs and exact compact solutions of lattice models seem to be rare and instable. By the numerical approximation of several examples on lattices [1, 2, 4], we emphasize that to have reliable information on the evolution of compact structures in physical systems is necessary to use a numerical method (e.g. [3]) preserving conservation laws (as energy) and also to check other quantities (as moments) related to the qualitative behavior of the solution.

The present research is supported by the PRIN2004 project *Modelli Matematici per la Dinamica del DNA*.

References

[1] J. C. Comte, *Exact discrete breather compactons in nonlinear Klein-Gordon lattices*, Phys. Rev. E **65**, N. 067601, (2002),1–4.
[2] S. Dusuel, P. Micheaux, M. Remoissenet *From kinks to compactonlike kinks*, Phys. Rev. E **57**, N. 2, (1998), 2320–2326.
[3] E. Hairer, C. Lubich, *Symmetric multistep methods over long times*, Numer. Math. **97**, (2004), 699–723.
[4] Y. Kivshar, *Intrinsic localized modes as solitons with compact support*, Phys. Rev. E **48**, N. 1, (1993), 43–45.
[5] P. Rosenau, J. M. Hyman, *Compactons: solitons with finite wavelength*, Phys. Rev. Lett. **70**, N. 5, (1993), 564–567.

[6] G. Saccomandi, *Elastic rods, Weierstrass' theory and special travelling waves solutions with compact support*, Int. Journ. Nonlin. Mechan. **39**, (2004), 331–339.
[7] L. V. Yakusevich, Nonlinear Physics of DNA, John Wiley & Sons Ltd, 1998.

Minimal modelling of DNA thermal and mechanical instabilities

Nikos Theodorakopoulos

The thermal and mechanical instabilities of double-stranded DNA (commonly known as "thermal melting" or "thermal denaturation" and "mechanical unzipping", respectively) share many of the properties of ordinary thermodynamic phase transitions; accordingly, they can be described in terms of a simple lattice model, which treats DNA at a mesoscopic level, assigning a single degree of freedom to describe the state of each base pair. The dynamics of base pair separation can be formulated in terms of a one-dimensional Hamiltonian which incorporates (i) the tendency of neighboring base pairs to be in a similar state (stacking interaction) and (ii) the local potential which describes hydrogen bonding that tends to bind each base pair. Typically this is represented by the Peyrard-Bishop-Dauxois[1] Hamiltonian

$$H = \sum_{n=0}^{M} \left[\frac{p_n^2}{2} + W(y_n, y_{n+1}) + V(y_n) \right] \tag{1}$$

which describes the transverse dynamics of M base pairs of unit reduced mass coupled to their nearest neighbors via a nonlinear spring $W(y_n, y_{n+1}) = [1 + \rho e^{-\alpha(y_{n+1}+y_n)}](y_{n+1} - y_n)^2/(2R)$ of range $1/\alpha$. The on-site potential is of the Morse type, i.e. $V(y) = (e^{-y} - 1)^2$.

The equilibrium statistical mechanics of the model is described by the partition function whose nontrivial, configurational part is given by

$$Z = \int dy_1 \int dy_2 \cdots \int dy_M K(y_1, y_2) K(y_2, y_3) \cdots K(y_{M-1}, y_M) \tag{2}$$

where $K(x, y) = e^{-W(x,y)/T - V(x)/T}$ and T is the temperature. It can be shown that in the thermodynamic limit $M \to \infty$ the free energy per site $f = -T \ln Z/M$ is equal to the smallest eigenvalue ϵ_0 of the integral eigenvalue equation

$$\int_{-\infty}^{\infty} \tilde{K}(x, y) \phi_\nu(y) = e^{-\epsilon_\nu/T} \phi_\nu(x) \tag{3}$$

where the symmetrized kernel $\tilde{K}(x, y) = [K(x, y)K(y, x)]^{1/2}$ is not of the Hilbert-Schmidt type. As a result, the integral equation (3) is singular, and the usual statements about non-degeneracy of the eigenvalue spectrum cannot be made. It is exactly this property which makes the type of Hamiltonian (1) relevant to true thermodynamic singularities in one spatial dimension.

In the absence of exact results on the possible non-analyticities of the spectrum of (3) the following approaches have been shown to be fruitful:

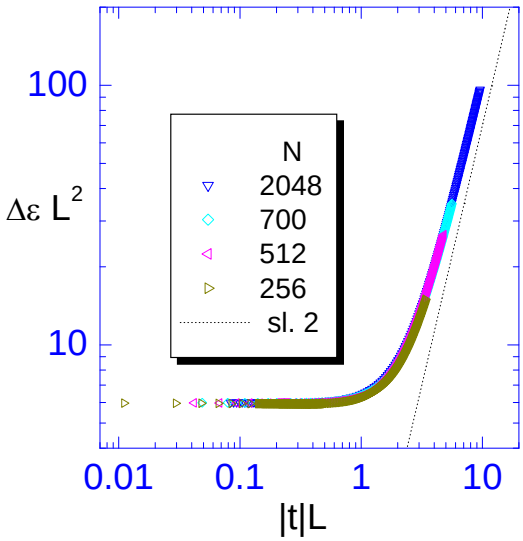

FIGURE 1. Finite-size scaling of the gap between the two lowest eigenvalues of (3).

A. finite-size scaling [3]: The integral in (3) has been approximated by Gauss-Hermite quadratures. This allows the integral equation to be viewed as a limiting sequence of symmetric matrix eigenvalue problems. It is then possible to follow the eigenvalue spectrum, and in particular the gap $\Delta\epsilon$ between lowest and next-to-lowest eigenvalues as a function of temperature, for a variety of Gauss-Hermite grids. As the number N of grid points grows, so does the effective transverse size of the system $L \sim 2N+1$. The analysis suggests that, as $L \to \infty$, the gap vanishes at a particular temperature T_c. Moreover, the values of the gap at finite L (cf. Fig. 1) exhibit finite-size scaling behavior of the type

$$\Delta\epsilon(L,T) = L^{-2} f_G\left(L|t|\right) \quad , \tag{4}$$

where $t = (T - T_c)/T_c$, $f_G(0) = const$, $f_G(x) \propto x^2$ if $x >> 1$, and as a result, $\Delta\epsilon_\infty(t) \propto |t|^\nu$ with $\nu = 2$. Further details on the finite-size scaling behavior of the thermodynamic properties of the model have been reported in [3].

B. Local equilibria and their stability properties [4]: The equilibria $\{y_n^{(\alpha)}\}$ of (1) can be obtained from a two-dimensional map which, in the case of $\rho = 0$, is of the form

$$\begin{aligned} p_{n+1}^{(\alpha)} &= p_n^{(\alpha)} + RV'(y_n^{(\alpha)}) \\ y_{n+1}^{(\alpha)} &= y_n^{(\alpha)} + p_{n+1}^{(\alpha)} \quad ; n = 0, 1, \cdots, M \end{aligned} \tag{5}$$

and has a single hyperbolic fixed point (FP) at $(p^{(0)} = y^{(0)} = 0)$. Fig. 2 shows the stable equilibria obtained under fixed transverse length boundary conditions, i.e. $y_0 = 0$, $y_{M+1} = L = 80$, and their total energies. These exact nonlinear structures can be thought of as domain walls (DWs), "interpolating" from bound to unbound phase.

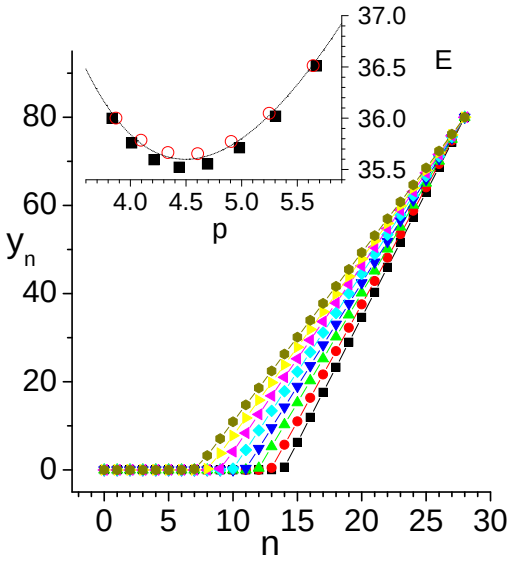

FIGURE 2. The 8 stable equilibria corresponding to $M = 28$, $y_0 = 0$, $y_{M+1} = L = 80$. Inset: total energies for both stable (filled squares) and unstable (open circles) equilibria. The continuous curve corresponds to a theoretical estimate.

It is possible to calculate the total energy and entropy which correspond to the global minimum under conditions $y_0 = 0$, $y_{M+1} = L = 80$, and subtract them from the corresponding energy and entropy, respectively, which correspond to the hyperbolic FP. The resulting free energy difference is - to lowest order in a low temperature expansion - of the form

$$\Delta G \propto [2 - T\sigma(R)]L \quad , \tag{6}$$

where $\sigma(R)$ reflects the differences between the frequency spectra of bound phase (optical phonons around the FP) and unbound phase (acoustical phonons around the flat top of the Morse potential). Eq. (6) suggests that at a temperature $2/\sigma$ spontaneous unzipping (thermal denaturation) occurs as the free energies of FP and and DW of minimal energy become equal. The above estimate of the critical temperature can be improved[4]; lowest-order perturbation theory gives a result which differs by less than 1% from the one obtained by finite-size scaling.

The picture which emerges from (A) and (B) above is consistent with the general argument by Landau which prohibits macroscopic coexistence of two phases at any $T \neq 0$ in 1D-systems, *provided that the energy E of the interface (DW) between the two phases is finite*, by showing that the system splits into a macroscopic number $MTe^{-E/T}$of domains. The argument does not apply to the class of systems discussed here, where energies and entropies of the DW are of order L, the maximum transverse displacement. It turns out that this is exactly the form of pathology needed to produce a phase transition in 1D.

References

[1] M. Peyrard and A.R. Bishop, *Statistical Mechanics of a Nonlinear Model for DNA Denaturation*, Physical Review Letters **62**, 2755-2758 (1989);

[2] T. Dauxois, M. Peyrard and A. R. Bishop, *Entropy driven DNA denaturation*, Physical Review E **47**, R4 (1993).

[3] N. Theodorakopoulos, *Thermodynamic instabilities in one dimensional particle lattices: a finite-size scaling approach*, Physical Review E **68**, 026109 (2003).

[4] N. Theodorakopoulos, M. Peyrard and R.S. MacKay, *Nonlinear structures and thermodynamic instabilities in a one-dimensional lattice system*, Physical Review Letters **93**, 258101 (2004).

Reporter: Giuseppe Saccomandi

Participants

Prof. Dr. Paolo Biscari

Dipartimento di Matematica
Politecnico di Milano
Piazza Leonardo da Vinci, 32
I-20133 Milano

Prof. Dr. Huajian Gao

Max-Planck-Institut für Metallforschung
Heisenbergstr. 3
70569 Stuttgart

Prof. Alain Goriely

Department de Physique; LP5
Ecole Normale Superieure
24, rue Lhomond
F-75230 Paris Cedex 05

Prof. Dr. Matthias Heil

Department of Mathematics
The University of Manchester
Oxford Road
GB-Manchester M13 9PL

Prof. Dr. Jacques Huyghe

Biomedical Engineering
Materials TEchnology
Eindhoven University of Technology
P.O. Box 513
NL-5600 MB Eindhoven

Prof. Dr. Ellen Kuhl

Lehrstuhl für Techn. Mechanik
T.U. Kaiserslautern
Erwin-Schrödinger-Straße
67663 Kaiserslautern

Prof. John H. Maddocks

Institut Mathematiques B
Ecole Polytechnique Federale
de Lausanne
CH-1015 Lausanne

Kamyar Malakpoor

Department of Mathematics
Eindhoven University of Technology
Postbus 513
NL-5600 MB Eindhoven

Prof. Dr. Andreas Menzel

Lehrstuhl für Techn. Mechanik
T.U. Kaiserslautern
Erwin-Schrödinger-Straße
67663 Kaiserslautern

Dr. Sebastien Neukirch

Laboratoire de Modelisation en
Mecanique, CNRS, Universite
P. et M. Curie, T.55-65, 4eme etage
4, Place Jussieu
F-75252 Paris Cedex 05

Prof. Dr. Ray W. Ogden

Department of Mathematics
University of Glasgow
University Gardens
GB-Glasgow, G12 8QW

Dr. Giuseppe Saccomandi

Dipartimento di Ingegneria
dell'Innovazione
Universita di Lecce
Via per Monteroni
I-73100 Lecce

Prof. Dr. Ivonne Sgura

Dipartimento di Matematica
Universita degli Studi di Lecce
Via Arnesano - C.P. 193
I-73100 Lecce

Prof. Dr. Nikos Theodorakopoulos

Theoretical& Physical
Chemistry Institute
National Hellenic Res. Foundation
Vasileos Constantinou 48
11635 Athens
Greece