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Progress in Industrial Mathematics at ECMI 2008

With 360 Figures, 109 in color and 46 Tables

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Preface

The 15th European Conference on Mathematics for Industry was held in the agreeable surroundings of University College London, just 5 minutes walk from the British Museum in the heart of London, over the five warm, sunny days from 30 June to 4 July 2008. Participants from all over the world met with the common aim of reinforcing the role of mathematics as an overarching resource for industry and business.

The conference attracted over 300 participants from 30 countries, most of them participating with either a contributed talk, a minisymposium presentation or a plenary lecture. 'Mathematics in Industry' was interpreted in its widest sense as can be seen from the range of applications and techniques described in this volume. We mention just two examples. The Alan Tayler Lecture was given by Mario Primicerio on a problem arising from moving oil through pipelines when temperature variations affect the shearing properties of wax and thus modify the flow. The Wacker Prize winner, Master's student Lauri Harhanen from the Helsinki University of Technology, showed how a novel piece of mathematics allowed new software to capture real-time images of teeth from the data supplied by present day dental machinery (see ECMI Newsletter 44).

The meeting was attended by leading figures from government, business and science who all shared the same aim – to promote the application of innovative mathematics to industry, and identify industrial sectors that offer the most exciting opportunities for mathematicians to provide new insight and new ideas. The finance day in the Lloyd's building provided an alternative venue and different talk themes. The panel discussions and the conference dinner generated formal and informal interaction and wide ranging discussions.

The organizing committee is grateful to all those who helped to make the meeting so successful. We thank Professor Frank Smith and University College London for the provision of the venue, Lord Hunt and Arren Ariel of the Lighthill Institute of Mathematical Sciences, and David Youdan and Amy Marsh of the Institute of Mathematics and its Applications for all their

effort in organizing the smooth running of the conference. We are very grateful to all our sponsors for their financial support (see: www.ecmi2008.org), and, in particular, Dr Robert Leese and the KTN for Industrial Mathematics for their help with the design work. The editors Alistair Fitt, John Norbury, Hilary Ockendon and Eddie Wilson thank Anthony Lock for his invaluable help with the publishing of these Proceedings.

Finally, a big thank you to all our participants who share the ECMI vision of using mathematics to make a better future in Europe – we hope this publication will help in the process of achieving this goal.

Oxford, *John Norbury (Chair)*
April 2009 *On behalf of the Organizing Committee*

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Modelling Living Tissues: Mechanical and Mechanobiological Aspects

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Summary. Mechanical modeling of living tissues is currently one of the most crucial challenges in research for mechanical engineers and mathematicians. Mechanics is a key factor to understanding the mechanisms that regulate many biological processes, such as mitosis, migration, and differentiation. This work aims to present the most crucial aspects, in the authors' opinion, to approach this challenge.

1 Introduction

"Classical science is a conversation between theory and experiment" [1]. However, nowadays, computer simulation has been recognized as a key tool for scientific research. Some of the most useful applications of computational modelling belong to Biology [2], and specifically to modelling living tissues with a structural function, supporting and transferring loads and moving other organs [3].

In fact, Mechanics has a strong influence on many biological processes characteristics of living tissues, such as, regulation of different biological processes (homeostasis), morphological and structural adaptation or tissue damage and repair, and it is responsible directly or indirectly of many diseases such as scoliosis, osteoporosis, malaria, etc. This fact has motivated that a wide number of research works have been recently developed with the purpose of modelling the active and passive behaviour of living tissues. Modelling the functional mechanical behaviour of living tissues has historically followed two approaches: (1) considering living tissues as inert structural materials, only dealing with Mechanics and (2) considering the biological reaction of living tissues to mechanical strains/stresses and the associated changes in microstructure and therefore in the mechanical behaviour itself.

The first field corresponds to classical *Biomechanics* and applies the principles of Mechanics to predict the mechanical behaviour (movement, strains and stresses) of a tissue or an organ, taking into account the acting loads, its microstructure and the external boundary conditions. The second one,

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known as *Mechanobiology*, tries to predict the evolution of the microstructure and biological constitution of a tissue or an organ as consequence of the mechanical environment.

In both cases, however, computational modelling presents strong difficulties that are necessary to keep in mind:

- We have to deal with very complex geometries that are sometimes evolutive. Therefore, computational geometry, medical imaging and data visualization are complementary tools.
- Most tissues involve large displacements and strains and internal material constraints which require sophisticated computational and mechanical models.
- Loads, boundary conditions and interactions are usually not known and very complex, which imply the need of accurate and complex experimental protocols to estimate them.
- Living tissues are regulated by multiple biophysical stimuli, thus, coupled fields (Multiphasic Mechanics, Biology, Chemistry) with very different time scales have to be modeled.
- Living tissues are hierarchically structurally composed materials, with their macroscopic properties depending on the different spatial scales involved. Therefore, a multiscale analysis is usually required.
- In contrast to usual engineering materials, living tissues have been optimally designed by the blind force of natural selection and show the remarkable ability to adapt not only their material properties and geometry, but also their functionality to environmental changes. Consequently, living tissues are evolving materials.
- Available experimental data present a strong variability that complicates the estimation of the parameters of the model, sometimes requiring stochastic approaches.

2 Biomechanical Tissue Modelling

Traditionally, Biomechanics in tissue modelling has been divided into two main fields of application due to the main characteristics of each tissue: hard and soft tissues.

On one hand, hard tissues typically undergo small deformations and behave nearly elastically in the range of interest. The first rigorous mathematical models for biological tissues that were introduced in the mid-1970s mainly addressed hard tissues such as bone [4].

The first modelling works of bone were elastic. For example, several authors try to model its mechanical behaviour through a mixture rule: Voigt's model [5] or Reuss's model [6]. Wagner and Weiner [7] modelled bone considering a composed material defined by its microstructure. Several authors [8, 9] proposed experimental correlations that define the mechanical properties assuming isotropic behaviour as a function of the apparent density. However, bone is a porous and anisotropic material. Therefore, additional, correlations have been proposed including the directional influence of the microstructure through the so-called "fabric tensor" [10–14]. More recently, poroelastic models have been proposed to model the complex behaviour of bone and the interaction with the fluid that flows within its pores, lacunae and canaliculi [15–19].

On the other hand, biomechanics models for soft tissues needs a more sophisticated theory involving geometrically non-linear approaches [20, 21]. Soft tissues have a non-linear stress-strain behaviour, and many of them are viscoelastic and highly incompressible. Most models consider hyperelastic anisotropic theories with different types of strain energy density functions (polynomial, exponential, stochastically-based). Polyconvexity considerations; internal constraints (incompressibility); linear and strain-dependent viscoelasticity; residual stresses; damage; and in some case (muscular tissue) coupled electro-mechanical active behaviour are only a few of the topics addressed when dealing with the structural constitutive behaviour of soft tissues [20–25].

3 Mechanobiological Tissue Modelling

The main aim of mechanobiological models is to evaluate how a mechanical stimulus can regulate biological mechanisms, such as, remodelling, healing, etc. Therefore, these models allow improving our understanding of how tissues react to changes in the mechanical environment. In this sense, there are two main approaches: phenomenological and mechanistic.

Phenomenological models are able to predict the long-term behaviour of a biological tissue under physiological and pathological loads by establishing direct relations between external causes (mechanical stimuli) and external effects (internal microstructure or morphology) without considering the intermediate actors as they are the cells.

Mechanistic models, on the other hand, try to unravel the mechanotransduction mechanisms that regulate tissue reactions, such as: how tissues interact with cells; how cells sense strain (mechanosensing); how cells express biochemical substances after sensing strain (mechanotransduction); and how individual cells communicate with each other (signalling).

3.1 Phenomenological-Based Approaches

Phenomenological models are particularly useful to predict the adaptive tissue changes regulated by mechanical factors without information of how cells actually do it. In this sense, these models have been used to solve some important engineering problems like improving implant design [26, 27], clinical therapies evaluation [28] or tissue engineering applications [29].

3.2 Mechanistic-Based Approaches

Mechanistic models try to incorporate the effect that cells exert on the evolution of the microstructure, accounting for processes like cell proliferation, differentiation, extracellular matrix production, etc. Although very difficult to validate, they are much more bio-physical and allow checking different hypotheses and design new experiments useful for a better understanding of the specific problem analyzed. Multiphasic formulations are usually used, including complex interactions between Mechanics, cells and volume growth in the framework of open systems [30, 31].

As for as the authors know, the most general mechanistic model that considers coupled equations between multiphasic and multicellular tissue mixtures in a continuum setting has been proposed by Doblare and García-Aznar [32]. This model incorporates different and crucial factors to achieve this goal: multiple species and different types of cells; sources, sinks and diffusion of both mass and cells; possible energy transfer between the different species and cells; tissue growth, differentiation, remodeling and damage; cell proliferation, migration, differentiation and necrosis.

This formulation has been particularized to different biological processes, such as, bone tissue adaptation [33] (see Fig. 1), bone healing [34, 35] (see Fig. 2) or cell migration [36].

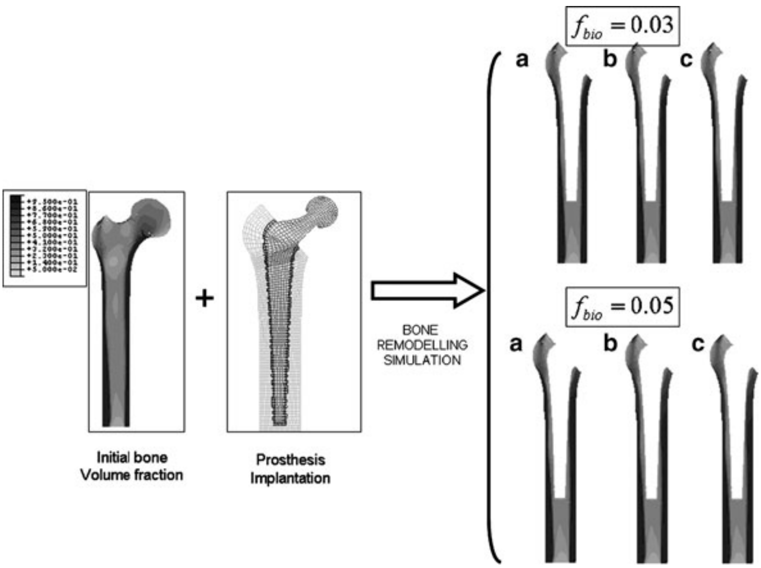

Fig. 1. Numerical simulation of the long-term adaptation process of a 2D model of a femur after implantation. Evolution of the bone volume fraction distribution for different biological factors and for different periods of time: (**a**) 330, (**b**) 660 and (**c**) 990 days [32]

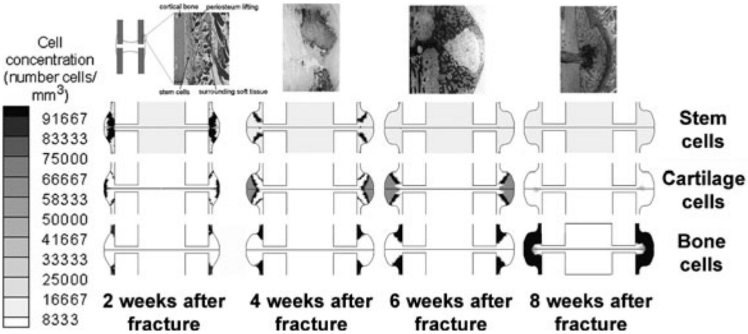

Fig. 2. Cellular distributions at different times of the healing process [32]: numerical results and histological sections (histologies taken from van der Meulen, Cornell University, NY; Sarmiento and Russell `http://www.hwbf.org/ota/bfc/index.htm`, 2002)

4 Conclusions and Further Work

Computational models including multi-scale and multi-physics approaches are a promising tool to better understand complex biophysical processes and are also essential in the growing field of quantitative and "evidence-based" Medicine. In fact, this kind of models allows exploring mechanotransduction at the cellular level and carry the information all the way up to the organ scale [4]. While the cellular scale can provide new insight into the fundamental mechanisms and help to explain signalling pathways (closer to biologists), large scale are essential to successfully address clinical and engineering problems.

Although these numerical techniques do already exists, their computational cost is still very high and the underlying biophysics is still not fully understood, so we are not able yet to fully analyze with sufficient confidence and accuracy a tissue at all the different scales incorporating all the relevant biophysical stimuli.

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New Mathematical Approaches for Image Reconstruction in the Oil and Medical Industries

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Summary. The problem of reconstructing images from measurements at the boundary of a domain belongs to the class of inverse problems. Although in different applications the techniques used to create the images work under different physical principles and map different physical parameters, they all share similar mathematical foundations. I will present here two mathematical approaches for image reconstruction. The first one is used to solve the so called history matching problem in the oil industry, and the second one is specially designed for the application of optical molecular imaging in biomedicine.

1 Introduction

Imaging is a broad field which covers all aspects of the analysis, modification, compression, visualization, and generation of images. There are at least two major areas in imaging science in which applied mathematics has a strong impact: image processing, and image reconstruction. In image processing the input is a (digital) image such as a photograph, while in image reconstruction the input is the data gathered on the boundary of an object. In the latter case, the data is limited, and its poor information content is not enough to generate an image to start with.

Image processing techniques apply numerical algorithms to either improve a given image or to extract information about the image [1]. Image segmentation is typically used for the latter purpose. It refers to the process of partitioning an image into multiple regions (locating objects and boundaries) in order to simplify its representation for its further analysis. Each region shares the same properties or characteristics such as color, intensity or texture. Different techniques have been applied for image segmentation. We mention here, graph partitioning methods in which the image is modelled as a graph; level-set methods in which an initial shape is evolved towards the object boundary; and statistical methods in which we view a region of an image as one realization of a random process (probability distribution functions and

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histograms are used to estimate the characteristics of the regions). We will not discuss the mathematics of image processing here.

On the other hand, image reconstruction refers to the techniques used to create an image of the interior of a body from data collected on its boundary [2]. Mathematically, an image reconstruction can be seen as the solution of an inverse problem in which the cause is inferred from the effect. We will show here two different applications in the oil and medical industries. The first application is the so called history matching problem where we want to estimate the unknown properties of a reservoir, such as its porosity and permeability, from the production data. We will apply to this problem an adjoint technique. The second application is the inverse fluorescent source problem in optical molecular imaging. We obtain here explicit solutions for a point source and a voxel source from which we estimate the location, size and total strength of a general source.

The goal of this paper is to illustrate the role of the imaging techniques in these applications. In the oil industry, for example, they improve our ability to design a good management strategy to increase the productivity and life of a reservoir. They help to better understand the reservoir behavior so that its performance can be predicted and controlled with higher reliability. On the other hand, in the biomedical application of optical molecular imaging they are used to monitor cellular and structural changes associated with predisease states such as dysplastic progression.

2 Reservoir Characterization

Oil fields typically extend over large areas, possibly several hundred kilometers across and full exploitation entails multiple wells scattered across the area. Initially, the natural differential pressure displaces hydrocarbons from the reservoir, into the wellbore and up to the surface. This is the primary recovery stage. As oil production takes place, the reservoir pressure declines, and eventually, the primary recovery stage reaches its limit. Typically, only a small fraction, around the 15% of the initial oil in place is produced during the primary recovery stage. During the second stage, water is injected into the production zone to sweep the oil from the reservoir. The secondary recovery stage reaches its limit when the injected fluid is produced in considerable amounts at the production wells and the production is no longer economical. Around 40% of the field's oil is produced during this stage. The third stage of oil production uses sophisticated techniques that alter the original properties of the oil. Its purpose is to improve oil displacement or fluid flow in the reservoir. It allows another 10% of the filed's oil to be recovered.

We consider here the case of 'secondary recovery' where water is injected through several injection wells conveniently located in order to enhance oil production. Potential problems associated with waterflood techniques include