6th International Workshop of Young Researchers on the Mechanics of Materials and Structures

Organizers: Antonio DeSimone* & Maurizio Angelillo**

* *International School for Advanced Studies, SISSA, Trieste*
** *Laboratorio di Strutture, Dipartimento di Ingegneria Civile, University of Salerno*

Venue

October 22-24 2014 at SISSA - International School for Advanced Studies
via Bonomea 265, 34136 Trieste, Italy
http://people.sissa.it/~desimone/iWeb/YRMMS14/Welcome.html

Minicourse on *Cell Mechanics* (6 lessons of 45 minutes each)

Prof. Robert McMeeking - University of California Santa Barbara
Mechanics, contractility, adhesion, signaling & cytoskeletal remodeling in cells

Invited speakers (talk of 45 minutes + 30 minutes for discussion)

22/10	Dr. Alessandro Lucantonio - SISSA, Italy *Asymptotic solutions for the shape design of swelling gels*
23/10	Dr. Róbert Nagy - University of Budapest, Hungary *A novel approach for estimating rupture risk of abdominal aortic aneurysms: in vivo material parameter identification via inverse isogeometric analysis*
23/10	Dr. Adrien Lefieux - University of Pavia, Italy *On the use of anisotropic triangles in an immersed finite element approach with application to fluid-structure interaction problems*
23/10	Dr. Diego Misseroni - University of Liverpool, UK *Tensile buckling, multiple bifurcations and Eshelby-like forces in elastic structures*
24/10	Dr. Davide Grazioli - University of Brescia, Italy *Multiscale modeling of multiphysics processes in Li-ion battery cells*

Scientific committee

Prof. Antonio DeSimone - SISSA, Trieste
Prof. Maurizio Angelillo - University of Salerno, Italy

Local organizing committee

Dr. Giovanni Noselli, Prof. Antonio DeSimone

Schedule of the workshop:

Wednesday, October 22 (meeting room, floor 7)

14.30 – 15.00	Welcome by the Director of SISSA Guido Martinelli and Antonio DeSimone
15.00 – 16.30	First and second lecture by Prof. Robert McMeeking - UCSB
16.30 – 17.00	Coffee break
17.00 – 17.45	Lecture by Dr. Alessandro Lucantonio - SISSA, Italy *Asymptotic solutions for the shape design of swelling gels*
17.45 – 18.15	30 minutes for questions and discussion
20.30	Social Dinner

Thursday, October 23 (room 5, ground floor)

09.45 – 11.15	Third and fourth lecture by Prof. Robert McMeeking - USCB
11.15 – 11.45	Coffee break
11.45 – 12.30	Lecture by Dr. Róbert Nagy - University of Budapest, Hungary *A novel approach for estimating rupture risk of abdominal aortic aneurysms: In vivo material parameter identification via inverse isogeometric analysis*
12.30 – 13.00	30 minutes for questions and discussion
13.00 – 14.30	Lunch
14.30 – 15.15	Lecture by Dr. Adrien Lefieux - University of Pavia, Italy *On the use of anisotropic triangles in an immersed finite element approach with application to fluid-structure interaction problems*
15.15 – 15.45	30 minutes for questions and discussion
15.45 – 16.15	Coffee break
16.15 – 17.00	Lecture by Dr. Diego Misseroni - University of Liverpool, UK *Tensile buckling, multiple bifurcations and Eshelby-like forces in elastic structures*
17.00 – 17.30	30 minutes for questions and discussion

Friday, October 24 (room 5, ground floor)

09.45 – 11.15	Fifth and sixth lecture by Prof. Robert McMeeking - USCB
11.15 – 11.45	Coffee break
11.45 – 12.30	Lecture by Dr. Davide Grazioli - University of Brescia, Italy *Multiscale modeling of multiphysics processes in Li-ion battery cells*
12.30 – 13.00	30 minutes for questions and discussion
13.00 – 13.15	Final discussion by the participants

Course by Prof. Robert McMeeking - University of California Santa Barbara

Mechanics, contractility, adhesion, signaling & cytoskeletal remodeling in cells

Cell mechanics is considered on the basis of the behavior of contractile stress-fibres consisting of long chains of actin cross-bridged by myosin motor proteins. These stress-fibres attach to complexes of proteins that include transmembrane molecules that bind to exterior ligands, and therefore adhere the cell to an extra-cellular matrix or to a substrate. External signals, e.g. from nervous impulses, and internally generated ones, such as arise when force is applied to cell adhesions, can trigger a cascade of chemical reactions that may remodel the cell cytoskeleton and the adhesions themselves. These processes can lead to the cell applying loads through its adhesions, with such forces being generated by the contractility of the cell. Furthermore, feedback from the response of the extra-cellular matrix or a substrate to which the cell is adhered can lead to different cell behavior depending on the stiffness of the external system. These aspects of cell behavior are known to play a role in development, in cellular behavior in healthy tissue, and in the response of cells during disease such as cancer and heart attacks. Bio-chemo-mechanical models for stress-fibre formation, remodeling and contractility will be presented. In addition, the formation and growth of adhesions will be considered, and signaling models, coupled to both the behavior of adhesions and the response of stress-fibres, will be developed.

Talks given by the participants:

Dr. Alessandro Lucantonio - SISSA, Italy

Asymptotic solutions for the shape design of swelling gels

The functionality of gel-based actuators, where the material swells and shrinks in response to changes in solvent content, critically depends on the capability of solving a shape design problem, which consists in determining the physical and geometrical properties of the system needed to obtain a prescribed target shape. Here, we study two prototypes of actuators: a thin elastomeric sheet under uniaxial pre-stretch that swells along its thickness, and a bilayer gel beam that bends upon swelling. We derive reduced models for both the systems, and we find semi-analytical formulas that may be employed for the solution of the shape design problem.

Dr. Róbert Nagy - University of Budapest, Hungary

A novel approach for estimating rupture risk of abdominal aortic aneurysms: In vivo material parameter identification via inverse isogeometric analysis

The diameter of a healthy infrarenal abdominal aorta measures between 15 mm and 24 mm. Abdominal aortic aneurysm is diagnosed, if a permanent and irreversible, localized spindle-shaped dilatation of the vessel is found, with diameter exceeding 1.5 times the value of the expected normal sate. The prevalence ratio in the population over the age of 50 years is 4-8% and 0.5-1% for men and women respectively. The rupture of these lesions is extremely hazardous, with fatal consequences in 80.2% of the cases. Although, due to modern regular screening tests, the deformations are often noticed at an early stage and the elective repair by open surgery or endovascular stent grafting can decrease the mortality ratio significantly, it still remains a high risk procedure: The thirty day operative mortalities are 4.3% and 1.8% respectively for the two methods with no significant difference between them in the long term.

In clinical practice, the decision on the management of aortic aneurysms is predominantly based on the diameter of the enlarged lumen (inner cross-section) and its rate of expansion. Although a good correlation is observed between these factors and the probability of failure, there is no exact causality between them. The possible rupture of untreated small aneurysms raised the demand

towards an improved decision strategy based on the stresses in the wall calculated by patient specific numerical modelling. One of the greatest disadvantages of these methods is the lack of individual calibration of the material parameters of the wall.

We introduce a novel method to measure the material parameters in vivo (in the living), thus, not only justifying the eligibility of the wall stresses, but also amending the analysis of the aneurysm by assessing the state of the material in the degradation process.

Using ECG-gated CTA images it becomes possible to follow the shape of the arterial wall through a complete cardiac cycle. Simulation of the blood flow, supported by the measurement of the blood pressure, provides the load field acting on the wall. The material model, connecting the known displacement and load fields, is established based on the wall microstructure and on biaxial macroscopic measurements. Finally, after developing an isogeometric finite element model, both the material model parameters are calibrated and the periodic displacement field is determined via a common weak-form variational principle capable to overcome the ill-posedness resulting from the initial lack of knowledge of the in plane deformations of the original problem.

Dr. Adrien Lefieux - University of Pavia, Italy

On the use of anisotropic triangles in an immersed finite element approach with application to fluid-structure interaction problems

The present work arises in the context of "immersed" methods. These methods are classically employed for problems involving interfaces, complex geometries, fluid-structure interaction, etc. They aim at overcoming meshing related issues. In this perspective, we first analyze several immersed strategies from the literature. A noticed crucial issue of such methods is that they often lack of accuracy. An envisaged accurate approach involves anisotropic triangles. Such elements are non-standard and many questions remain open among which their inf-sup stability within the mixed finite element method used for incompressible flows. The work performed involves numerical studies of several mixed finite elements for the incompressible Stokes problem featuring highly distorted triangles. Finally, an application to a fluid-structure interaction problem modeled by the incompressible Navier-Stokes equations for the fluid and a thin rigid leaflet for the solid is presented.

Dr. Diego Misseroni - University of Liverpool, UK

Tensile buckling, multiple bifurcations and Eshelby-like forces in elastic structures

Several 'unexpected' behaviours of elastic structures are given evidence both theoretically and experimentally. These include structural effects related to constraint's curvature and to the presence of configurational 'Eshelby-like' forces. In particular, the curvature of a constraint against which the end of an elastic rod is prescribed to move is shown to deeply influence bifurcation and post-critical behavior. Moreover, surprising phenomena and effects on stability are demonstrated as related to the presence of movable constraints, so that configurational forces are developed. It is theoretically shown and experimentally proven how both flexure and torsional deformation of an elastic rod confined into a perfectly smooth channel can provide a longitudinal propulsion. Two proof-of-principle devices have been realized, highlighting the concepts, namely, an elastica arm scale and a 'torsional gun'.

Dr. Davide Grazioli - University of Brescia, Italy

Multiscale modeling of multiphysics processes in Li-ion battery cells

In recent contributions the computational homogenization technique was tailored to model the

multiphysics processes that take place in Li-ion batteries. The formulation originally proposed in [1] has been recently extended [2] to take into account electroneutrality, quasi-static Maxwell equations, time dependent scale transitions, and scale separation in time. The approach described here originates from the fundamental balance laws (of mass, force, charge) at both scales and the multi-scale analysis roots itself on an energy-based weak formulation of the balance laws, which allows to extend the Hill-Mandel energy averaging theorem to the problem at hand. This note details the microscale formulation. Balance laws are accompanied by constitutive assumptions that emanate from a rigorous thermodynamic setting. After the discretization of the weak form and by advancing in time by the Backward Euler approach, a numerical algorithm has been implemented by means of Abaqus User Element (UEL) scripts. Several case studies have been simulated to validate the implemented formulation. The first [3] concerns a one-dimensional application to ionic transport in Li-ion batteries electrolyte, inspired by [4]. The second case study [5] simulates the charge/discharge process of an all-solid-state Li-ion battery. The numerical results have been compared with the outcomes of one-dimensional characterization derived in [6]. Finally the proposed theoretical framework is applied to a two-dimensional problem, with the aim of investigating the behavior of a multi phases microstructure [3].

[1] A. Salvadori, E. Bosco and D. Grazioli. A computational homogenization approach for Li-ion battery cells: Part 1 - formulation, Journal of the Mechanics and Physics of Solids 65, 114-137, 2014.

[2] A. Salvadori, D. Grazioli and M.G.D. Geers. Governing equations for a two-scale analysis of Li-ion battery cells. Under review for publication on International Journal of Solids and Structures.

[3] A. Salvadori, D. Grazioli, M. Magri, M.G.D. Geers, D. Danilov and P.H.L. Notten. A novel approach in modelling ionic transport in the electrolyte of (Li-ion) batteries. Submitted for publication in Journal of Electrochemical Society.

[4] D. Danilov and P.H.L. Notten. Mathematical modeling of ionic transport in the electrolyte of li-ion batteries. Electrochimica Acta, 53, 5569–5578, 2008.

[5] A. Salvadori, D. Grazioli, M. Magri, M.G.D. Geers, D. Danilov and P.H.L. Notten. A novel multi physics approach in modeling all solid state (Li-ion) batteries. Submitted for publication in Journal of Power Sources.

[6] D. Danilov, R.A.H. Niessen and P.H.L. Notten. Modeling all-solid-state li-ion batteries. Journal of The Electrochemical Society, 158, A215-A222, 2011.