Unravelling the link between cartilage microscopic structure and its exceptional lubrication properties

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Abstract
Cartilage, in essence a mixture of (free and cross-linked) polymers of different architecture imbibed in water, is an exceptional lubricant. In fact, it is able to provide very low friction between joints under a large variety of static and dynamical conditions and for normal pressures spanning various orders of magnitude. Despite its importance and years of extensive efforts in the bio-materials community, replacing damaged cartilage with a synthetic analogue is still an open problem (see *e.g.* [1]), since no man-made material has been able to mimic such properties. This should not really come as a surprise, considering that, apart from the broadly-accepted necessity of hydration, the microscopic mechanisms leading to such low friction are still poorly understood [2-4]. The key is to shed light on the lubrication mechanisms responsible for the frictional performances of the tissue, which is an extremely important element for the design optimisation of tissue mimics (see Fig. 1). The goal of this project is to systematically investigate, using particle-based coarse-grained molecular dynamics coupled to continuum-based meso-scale simulations (see *e.g.* [2,3]), the structure-(mechanical) properties relation in this system. More precisely, the goal is to understand the role of the various polymer architectures found in the mixture in determining friction in different regimes, thereby providing rational design principles to biomaterials scientists for the synthesis of cartilage analogues.

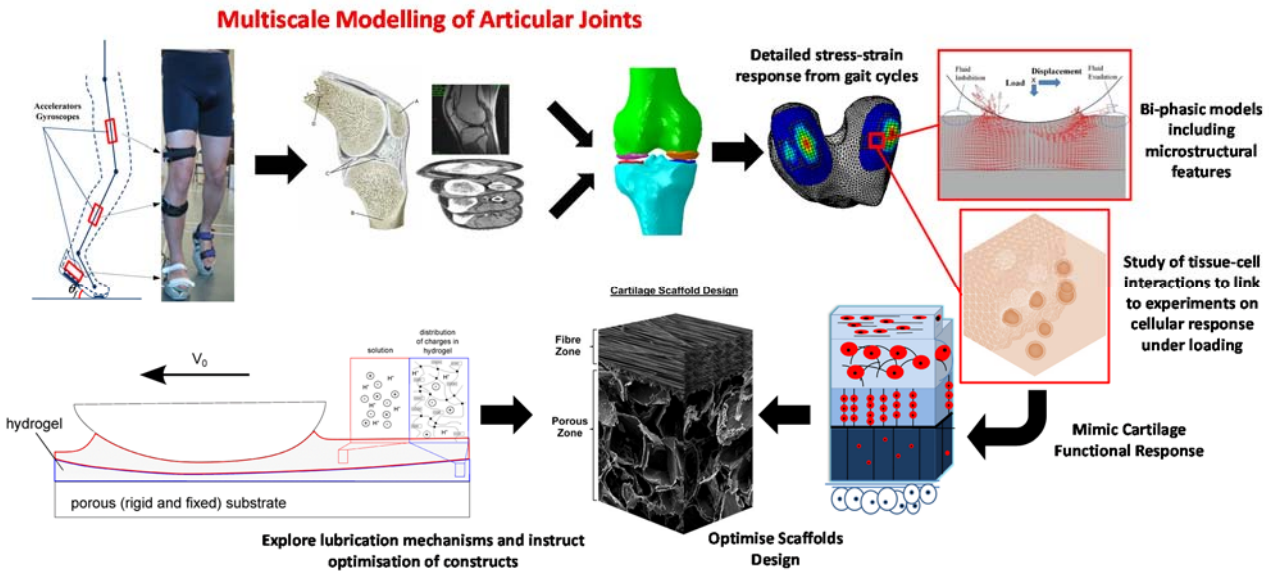

Figure 1. Strategy for modelling of articular joints across the scales. Focus here is the lubrication mechanisms

References

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[2] Accardi, M.A., Dini, D., Cann, P.M., 2011, Experimental and numerical investigation of the behaviour of articular cartilage under shear loading—interstitial fluid pressurisation and lubrication mechanisms. *Tribology International*, *44 (5)*, pp. 565-578.
[3] Mattei, L., Campioni, E., Accardi, M.A. and Dini, D., 2014, Finite element analysis of the meniscectomised tibio-femoral joint: implementation of advanced articular cartilage models, *Computer methods in biomechanics and biomedical engineering*, *17 (14)*, pp. 1553-1571.
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What is the multi-scale nature of the project?
At the nanoscale, (Non-equilibrium) Langevin dynamics simulations with a coarse-grained model are necessary to determine the mechanical properties of the system as a function of the polymer architecture and the type of stress. These can then be used as an input for a mesoscale Finite Element (FE) model of cartilage systems and real joints.

How do the expertises of the supervisors complement each other?
Dr. Angioletti-Uberti is an expert in molecular dynamics simulations and coarse-grained models of soft matter system. Prof. Dini has also a strong expertise in molecular dynamics simulations, in particular related to the determination of non-equilibrium properties for confined (generalised) fluids, and he is also a recognised leader in the field of mesoscale models for tribology, soft matter and biomechanics, thereby covering the larger scales.

Literature Review
Title: Molecular Dynamics simulations of polymer brushes under non-equilibrium conditions

Bibiliography:
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[3] Ewen, J.P., Gattinoni, C., Zhang, J., Heyes, D.M., Spikes, H.A. and Dini, D., 2017. On the effect of confined fluid molecular structure on nonequilibrium phase behaviour and friction. *Physical Chemistry Chemical Physics*, *19*(27), pp.17883-17894.

MSc Project
The student will start to build a coarse-grained model (with a similar coarse-graining approach as in [1-3] above) of the system and run non-equilibrium simulations under different shear rates and pressures to determine friction(shear rate, pressure) for different brush architectures. In particular, we will start with monodisperse polyelectrolyte brushes of linear and bottle-brush polymers, focusing on the role of polymer length and their ionisation degree and, for the branched structures, also the linear density and length of side arms. Simulations will be complemented with theoretical work on trying to address the observed numerical trends in terms of scaling laws for polymers.