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Fast Pre-Clinical *In-Silico* Surrogate Methods for Statistical Shape Modelling

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Introduction: In both industrial and clinical use, contemporary pre-clinical analysis methods place increasing emphasis on a more 'holistic' understanding of performance, accounting for a wider range of factors. This places a heavy time-burden on pre-clinical analysis methods, with wide-ranging stochastic methods, sweep studies or sensitivity analysis methods requiring extended processing time. In tension with this, there is an expectation that, in order to be practically useful, any computational support tool should be responsive, delivering results more quickly or even near-instantaneously for 'real-time' clinical use. The broad challenge is to make these models fast, accessible and relevant for end-users in a clinical and/or industrial context.

Traditional 'mechanistic' simulations (e.g. finite element analysis, FEA) offer good 'detail-modelling', but with high solve times. A different approach is required, particularly when statistical shape/intensity modelling (SSIM) of bones is used. Surrogate models do not directly reproduce the mechanics of the model, but instead find a simplified mathematical relationship to approximate the more complex simulator. Such models have already been demonstrated for the hip[1], knee[2], and foot[3], amongst others. Surrogate models trade faster performance for an associated loss in accuracy. This decrease in accuracy is important, and a good surrogate emulator should include some measure of the induced uncertainty (or 'error'). A previous study[1] treated the proximal femur as a single entity, returning one scalar parameter (e.g. mean or maximum) to represent the entire bone. By contrast, FEA provides much higher spatial resolution of local stress/strain variations. We investigate a compromise, in which the femur is partitioned into a smaller number of sub-sections, treated separately for the purposes of surrogate modelling (Fig.1). This provides a good trade-off between outputting more clinically relevant information, whilst minimising computational overhead.

Methods: An existing dataset[4] (static load-case on the intact/implanted proximal femur with a SSIM[5]) was used as the training set for a fast emulator. 500 pre-processed FEA solutions were

parsed to map out the design-space (35 PCA weights, 1 load-scaling term). A custom emulator was encoded using MATLAB (Mathworks, MA), to estimate both the mean-value and associated uncertainty for any given inputs within the convex hull of the design space. The output metric demonstrated is the mean change in strain between the intact and implanted cases (i.e. a single scalar value for each separate section). Results were visualised using 2D colour-coded GUI representations, with uncertainty also visualised using appropriate colour-coded highlighting.

Results: With 16 sections, different local trends could be distinguished (e.g. reduced strains within the head but increased strains in the neck) which are lost if values are 'averaged' by an emulator. Runtime was <2 seconds: close to instantaneous. However, the training set is sparse, with the Z-score distance between points generally >1 due to the high dimensionality (large number of factors). The 500 trials used are inadequate to give good coverage of the entire possibility space with such a large number of factors (coverage is <50% for first 4 factors, <1% for any more than 10 factors), implying more trials are needed for better accuracy.

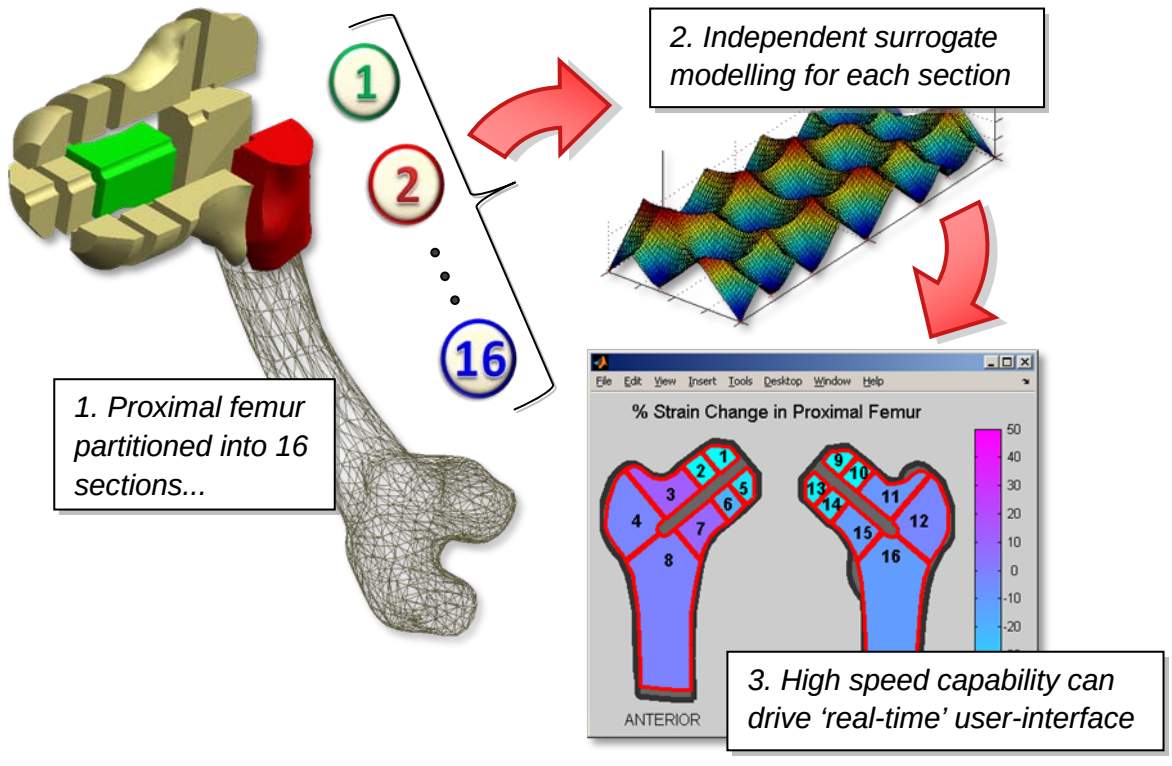

Fig.1: Surrogate model concept: 1) Proximal femur partitioned into sections to differentiate strain effects in different areas. 2) Independent high-speed emulators constructed for each section, providing rapid 'virtual' FEA prediction. 3) Results visualised in near 'real-time'.

Discussion: An initial 'real-time' emulator has been demonstrated for this particular femoral-resurfacing study. With further optimisations, solve time could be reduced. This may be necessary, because the present study is limited, neglecting dynamic load-cycle variations, mal-positioning, or detailed musculoskeletal loading. All of these factors will considerably increase the search-space, making fast surrogate modelling more challenging. Surrogate prediction uncertainty also becomes a problem as more factors are added and the spatial resolution is increased further. A larger pre-processed training set would be recommended for future work. However, this study clearly demonstrates the potential for fast surrogate models to deliver near instantaneous computational decision-support capabilities to the end-user in the industrial or clinical environment.

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