

An open-source tool for the validation of finite element models using three-dimensional full-field measurements

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Abstract

Three-dimensional (3D) full-field measurements provide a comprehensive and accurate validation of finite element (FE) models. For the validation, the result of the model and measurements are compared based on two respective point-sets and this requires the point-sets to be registered in one coordinate system. Point-set registration is a non-convex optimization problem that has widely been solved by the ordinary iterative closest point algorithm. However, this approach necessitates a good initialization without which it easily returns a local optimum, i.e. an erroneous registration. The globally optimal iterative closest point (Go-ICP) algorithm has overcome this drawback and forms the basis for the presented open-source tool that can be used for the validation of FE models using 3D full-field measurements. The capability of the tool is demonstrated using an application

example from the field of biomechanics. Methodological problems that arise in real-world data and the respective implemented solution approaches are discussed.

Keywords: 3D point-set registration; global optimization; digital image correlation (DIC); biomechanics; synthetic bone

1 Introduction

Computational models, in particular finite element (FE) models, are increasingly being used to understand and predict the behavior of complex biological systems, for which experimental measurements are to some extent impractical or even impossible. However, any model is only a simplified representation of the real world. For the model results to be (clinically) relevant, the limitations of the model must be figured out and according to the National Academies of Sciences, Engineering, and Medicine of the United States [1] and Viceconti et al. [2] three issues should be addressed in particular: verification (confirming that the implementation of the model has been done correctly and that the model equations are solved accurately), validation (determining how well a model represents the real world phenomena it is intended to predict), uncertainty quantification (determining how variations in the model affect its outcome). Validation is based on the statistical comparisons of the model's outcome and experimental measurements and if necessary, the model is modified in an iterative manner, e.g. by FE model updating [3], until the difference between the prediction of the model and measurements satisfies the requirements.

FE models are widely used in the field of biomechanics (e.g. [4]) and their validation is usually based on displacements and/or strains measured on the surface of a given object under load. For hard tissue, e.g. bone, strain gauges have been used for a long time [5]. Strain gauges are, however, only capable of measuring strains at single spots in regions with very low strain gradients and they reinforce materials with low Young's moduli [6] meaning strain readings can be error prone. Contactless three-dimensional (3D) full-field measurement methods such as digital image correlation (DIC) overcome these limitations [5][7] and allow for a more comprehensive and accurate validation [8]. A speckle pattern is applied to the surface of the object and during loading two cameras (or more) record images of the deforming object. The images are then divided into groups of pixels (pixel-subsets) and the pixel-subsets in a reference image are correlated to the same pixel-subsets in the following image in order to find the displacements for each subset center. Spatial differentiation of the displacements can then be used to derive strains [9-10].

Displacements and strains are computed and measured pointwise. The FE point-set includes the coordinates of the nodes of the mesh (FE points) and the DIC point-set includes the coordinates of the pixel-subsets (DIC points). It is essential that the statistical comparison is done based on the unloaded state of the object and that the point-sets are accurately registered in one coordinate system. Point-set registration is a non-convex optimization problem, in which the spatial transformation that minimizes the registration error has to be found. So far, the iterative closest point (ICP) algorithm [11] has widely been used to solve the problem (e.g. [12-14]). The ICP algorithm, however, requires a good initialization without which it easily converges on a local minimum associated with an erroneous registration. This drawback has been overcome by the globally optimal iterative closest point (Go-ICP) algorithm developed by Yang *et al.* [15].

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69 The Go-ICP algorithm forms the basis of the presented open-source tool that is developed for the
70 validation of FE models using 3D full-field measurements. To the best of our knowledge, no other
71 such tool has been made available yet. The validation of a biomechanical model using DIC based
72 displacement measurements is used to describe its underlying methodology and to demonstrate its
73 capability in a proof-of-principle analysis.

74

75 **2 Structure of the tool**

76 *2.1 Framework*

77 The tool is written in Matlab (MathWorks, USA; it was tested for R2014a and later versions) and
78 runs on every computer platform. It requires the data to be sorted in columns and since there is no
79 standardized data format across FE and full-field measurement software, the integrated import
80 function in Matlab was selected for data import. This allows the individual selection of data
81 independent from formatting and column order. From that point on, the user is guided through the
82 entire validation process by a GUI dialogue.

83

84 *2.2 Registration: Go-ICP*

85 The point-sets are centered and normalized to the $[-1,1]^3$ space as this is a prerequisite for the
86 Go-ICP algorithm. The Go-ICP algorithm is a combination of the well-known ICP algorithm and
87 the Branch-and-Bound (BnB) scheme and searches the spatial transformation that best aligns the
88 point-sets by minimizing the L_2 -norm of the closest-point residual vectors (registration error E).
89 Full details can be found elsewhere [15] but a brief description is given here.

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Input for the algorithm are the two centered and normalized point-sets, a registration error E set to infinity, and an arbitrary initial transformation described by a rotation matrix and a translation matrix. The BnB scheme starts by searching the space of $SE(3)$ for a transformation that gives an upper bound value of E which is lower than the current value of E . Having found a better transformation, the ICP algorithm is called and initialized with that transformation. The ICP algorithm then refines the transformation and the registration error E can be further decreased. This loop iterates until E has converged to its global minimum E^* . The convergence threshold $\varepsilon = aN$ depends linearly on the number N of points; a is the threshold factor. In the tool, the transformation domain to be explored by Go-ICP is set to $[-\pi, \pi]^3 \times [-1, 1]^3$.

For equal point-sets, the Go-ICP has been proven to work reliably [15]. However, for several reasons, point-sets obtained from real-world data are not equal and this is associated with an inherent registration error and the emergence of additional local minima of E that might be close to the global minimum E^* . Thus, in order to find E^* , the convergence threshold needs to be small. Starting out from a value of 0.001, the threshold factor a is iteratively decreased (0.0005, 0.0001, 0.00005, 0.00001, ...) until the registration error has converged to E^* . E is defined to be converged when the relative change between two consecutive iterations is between 0% and 5%. To make the registration process more robust to large closest-point distances (outlier), the tool also employs a trimming procedure [15, 16] that removes a given percentage of points with largest closest-point distances. Trimming is applied through a modification of the convergence threshold: $\varepsilon = a(1 - \rho)N$ and ρ is the trimming factor ranging from 0 (no points are removed) to 1 (all points are removed). The user can set ρ depending on the desired amount of points in the registration and ultimately in the statistical comparison.

2.3 Statistical comparison

After registration, computed and measured displacements are statistically compared. This can be done based on the original point-sets but the user is also given the opportunity to define a region of interest (ROI). The spatial resolution of the point-set is determined by the number of points in the given ROI. The point-set with lower spatial resolution is defined to be the primary point-set, the other one is defined to be the secondary point-set. Statistical comparison is then done between each displacement of the primary point-set and the averaged displacement of a surrounding point-cloud of the secondary point-set (averaging method) or between closest-point pairs (closest-point pair method). The point-cloud is bounded by a sphere around a given point of the primary point-set (Fig.1) and the radius of that sphere can be set in the original length unit; its normalization is done by the tool. No weighting is used for the averaging. In the case that no points lie within a given sphere, the respective basis point is not considered for statistical comparison. The user can decide whether to include only surface nodes or also nodes inside the given object depending on the chosen FE-point set.

Statistical comparison includes linear regression analysis with information about the coefficient of determination (R^2), the slope, and the offset of the best fit line. Furthermore, the mean absolute error (MAE), the mean absolute percentage error ($MAPE$), the root mean square error ($RMSE$), and the root mean square percentage error ($RMSPE$) are computed. This is in line with previous work on validations of biomechanical FE models [2][12][13][14]. The tool also provides a color-map on the primary point-set that shows the absolute difference between computed and measured displacements as in [8]. This is useful to identify regions with a good or bad agreement between

the model's outcome and measurements. Closest-point pairs are used for the computation of differences.

3 Proof-of-principle analysis

3.1 Material and methods

Exemplarily, a biomechanical FE model of a synthetic femur with a cemented hip implant was validated at a compressive load of 5 kN using DIC based displacement measurements. In particular, total displacements were chosen.

The specimen was prepared by an experienced surgeon and potted in a 10° angle in both the frontal and the sagittal plane [17] using a custom-made guide. Plastic steel epoxy (Devcon, USA) was used to pot the femur in a plastic cup (filling height of the epoxy: 65 mm, diameter of the cup: 100 mm, femoral condyles were in contact with the plastic cup). The cup was held by a stainless steel cylinder which was bolted upon a series of adjustable fixtures which were clamped onto the base of the mechanical testing machine (Dartec H10, Zwick Roell Group, GBR). Load was applied at the ball of the implant through a cylinder with a spherical hole whose diameter is 2 mm larger than the ball diameter (28 mm). Mechanical testing was displacement-controlled (Control Cube, Zwick Roell Group, GBR) with a displacement rate of 2 mm/s and load and displacement were recorded at 250 Hz. The synthetic human femur (#3403; Sawbones, USA) is made of short fiber filled epoxy resin (cortical bone) and solid rigid polyurethane foam (cancellous bone), the hip implant Exeter V40 (Stryker, GBR) is made of ultra-high strength stainless steel, the vacuum-mixed bone cement Optipac (Biomet, GBR) is made of polymethyl methacrylate.

DIC measurements were performed with the Q-400 system with two video cameras (resolution: 5 MP, frame rate: 10 fps) and the Istra 4D software (LIMESS Messtechnik und Software GmbH, GER). For calibration, the calibration plate GL-06-WMB_9x9 from the same company was used. Correlation parameters (subset size, spacing between the subset centers) were optimized by a variation study with the criterion of obtaining minimum measurement error. The measurement error was quantified by the total displacement averaged over all subsets for ten measurements without load (where theoretical total displacements are zero). Minimum measurement error (0.0057 mm) was obtained when the subset size was 19×19 pixels and spacing between the subset centers was 4 pixels. Two filters (local regression and smoothing spline) were tested but their improvement on the measurement error (4% and 6%) was negligible small so that none of them were applied. The optimized setting resulted in $N = 11376$ subsets in the ROI (Fig.2a).

The FE model was developed with reverse engineered geometries of the synthetic femur and the hip implant (SolidWorks, Dassault Systèmes, FRA). The design of the cement mantle and the positioning of the model parts were performed in line with X-ray images of the specimen. Linear elastic transversely isotropic material properties (Tab.1) were assigned for the synthetic cortical bone and linear elastic isotropic material properties (Tab.2) were assigned for the other model parts. Computations were performed with Abaqus 6.12 (Simulia, Dassault Systèmes, FRA). Modified second-order ten node tetrahedral elements (C3D10M) were used for meshing. A mesh sensitivity study was performed to find the number of elements in the mesh at which the total displacement converges. The FE-ROI was chosen to be similar to the DIC-ROI and the optimized mesh consists of 6284 surface nodes within the ROI (Fig.2b).

The spatial resolution of the FE point-set (6284 points/ROI) was lower than the DIC point-set (11376 points /ROI) and thus, the FE point-set was the primary point-set. The trimming factor ρ was set to 0 and 0.1. Statistical comparison was done based on the averaging method and the point-cloud radius was set to 1.0 mm.

3.2 Results

When performing the registration without the use of trimming, the registration error E first increased slightly and then decreased with decreasing threshold factor a until it finally converged to E^* : 9.47 ($a = 0.001$); 9.48 ($a = 0.0005$); 0.58 ($a = 0.0001$); 0.56 ($a = 0.00005$). The minimum registration error E^* was smaller (0.42) when trimming with a factor of $\rho = 0.1$ was used, but the number of iterations until convergence remained unaltered. Trimming reduced the number of available points for the statistical comparison to 5656 FE points and 10238 DIC. The registered point-sets that were trimmed with $\rho = 0.1$ were used for statistical comparison. The FE model predicted the measured total displacement with a coefficient of determination $R^2 = 0.85$, a slope of 0.80, and an offset of -0.33 mm. Errors were $MAE = 0.93$ mm, $MAPE = 30.60\%$ $RMSE = 0.04$ mm, $RMSPE = 42.18\%$, (Fig.3).

4 Discussion

We have introduced an open-source tool for the validation of FE models based on 3D full-field measurements. For optimum point-set registration regardless of the initialization the Go-ICP algorithm [15] was implemented and a GUI guides the user through the entire process. The validation of a biomechanical synthetic bone-implant model based on DIC based displacement

measurements was presented as an example to demonstrate the capability of the tool in a typical scenario.

We used total displacements in the validation example because they were deemed more reliable than strains for the purposes of assessing the capabilities of the tool. The derivation of strains can amplify errors contained in the displacements and in our case, large errors in strain measurements were observed, which we attributed to noise [7][10]. However, the tool can be applied in the same way to full-field strain measurements, which are generally more relevant for biomechanical studies [21-22]. Moreover, the tool is suitable for application in other fields, e.g. thermodynamics, in which FE models can be validated based on any kind of full-field measurements and furthermore, the tool can also be used for comparing the outcome of two models with different meshes as part of the verification and uncertainty quantification.

The Go-ICP algorithm has been proven to work reliably for equal point-sets [15] but point-sets derived from real-world data differ from each other although they describe the same object. This is e.g. because the sampling in full-field measurements cannot generate the exact same point-set that is obtained by meshing in the FE model and because of deviations between the mesh and the real object geometry. The setting of the convergence threshold becomes crucial because unequal point-sets are associated with additional local minima that may lie close to the global minimum of the registration error. Thus, we implemented a loop that decreases the convergence threshold stepwise until it is small enough that the global minimum can be found. Outlier robustness of the registration can be obtained by a trimming procedure [15-16]. However, as this procedure decreases the number of points available for the statistical comparison, we suggest a careful setting

of the trimming factor that gives a balanced trade-off between outlier robustness and amount of available data for the statistical comparison. In the given example, the number and size of outliers were small and thus, the registration error was not very sensitive to the trimming factor. After registration, the values of the given primary point-set are statistically compared with the averaged values of a surrounding point-cloud. This smoothing method was chosen to reduce the error that might be introduced by large differences between computed and measured values when the distance between a closest-point pair is high.

Perfect agreement between the model's outcome and full-field measurements would give a best fit line with the R^2 -value and the slope equal to 1 and the offset and the set of error measures equal to 0. However, in reality there are always errors. The main sources of errors in the FE model are the geometry modelling and meshing, the constitutive model, and the boundary conditions. The main sources of errors in full-field measurements depend on the particular application. This is, in DIC measurements, the speckle pattern, the image acquisition and digitalization, and the correlation parameter settings [5][7][10].

In the current study we have presented an open-source tool which can be used to validate FE models based on full-field measurements. The tool was developed to provide a method of easily linking computational and experimental research. Its capability has been tested in a typical scenario and future research will utilize the tool in various biomechanical studies.

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