Bayesian optimization-based inverse finite element analysis for atrioventricular heart valves

Colton J. Ross[1], Devin W. Laurence[2], Ankush Aggarwal[3], Ming-Chen Hsu[4], Arshid Mir[5], Harold M. Burkhart[6], and Chung-Hao Lee[1,7]

affiliations: [1] Biomechanics & Biomaterials Design Laboratory, School of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK, USA

[2] Children's Hospital of Philadelphia, Philadelphia, PA, USA

[3] Glasgow Computational Engineering Centre, James Watt School of Engineering, University of Glasgow, Glasgow, UK

[4] Department of Mechanical Engineering, Iowa State University, Ames, IA, USA

[5] Department of Pediatrics, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA

[6] Department of Surgery, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA

[7] Department of Bioengineering, University of California Riverside, Riverside, CA, USA

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correspondence: Chung-Hao Lee, e-mail: clee@ucr.edu

Supplemental Information 3 – Sub-Studies of Test Case 1: Inflation Testing

We also sought to understand the influence of segmentation errors (i.e., noise) and modeling assumptions on the objective surface and optimization convergence.

Sub-Study (I): Effects of Noise in the Obtained BO Solution

We generated artificial noise for the synthetic solution of the inflation test by adding randomly sampled values from a Gaussian (normal) distribution to the 3D Cartesian coordinates of the final deformed mesh. The noise-adjusted element centroid locations then served as the comparison point cloud. A range of noise levels were tested using Gaussian distributions with a mean of zero and standard deviations of 0.005, 0.01, 0.02 and 0.03 mm. We also performed BO for the scenario with a standard deviation noise level of 0.02 mm.

By testing the effects of additive noise in the inflation test comparison point cloud, we found that an increase in the additive noise (i.e., a larger standard deviation) resulted in a widening of the valley of nearly equivalent solutions (**Fig. S5**). The objective function values associated with the synthetic solution at each noise level, in increasing order, were found as 1.14 mm/mm, 2.39 mm/mm, 4.52 mm/mm, and 6.95 mm/mm. The widening of the valley of nearly equivalent solutions also caused a wider spread of parameter values in the Bayesian optimization performed at the 0.02 mm noise level (c_1 = 0.318±0.091 kPa and c_2 = 11.20±1.02 than in the case without additive noise, however, the range of objective function values were smaller ($\mathcal{F}$ = 18.21±0.01 mm).

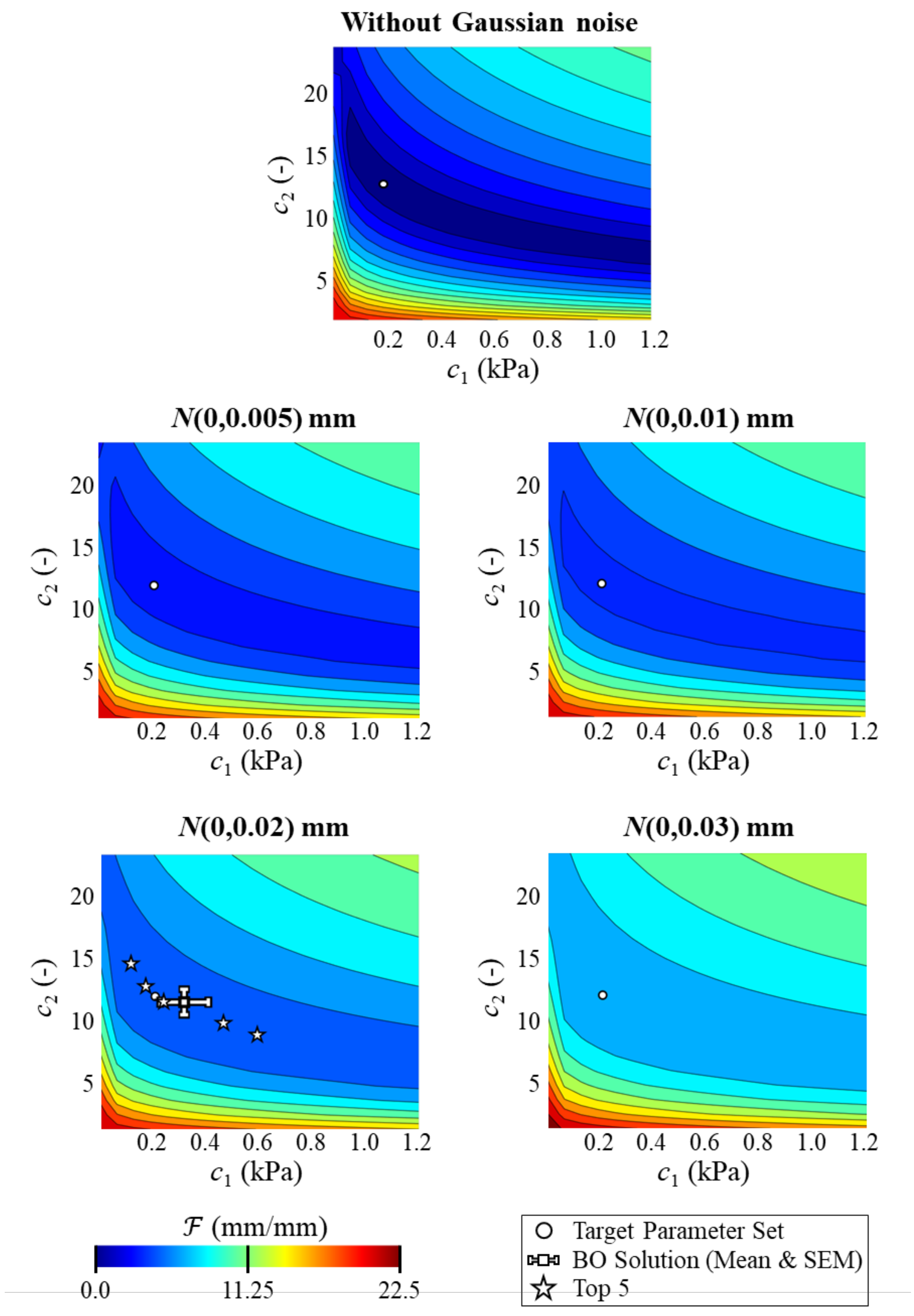

Figure S5: Contour plots and finite element meshes of the objective function surfaces considering different amounts of noise generated from a Gaussian distribution. The BO solution is shown for the case of $N(0,0.02)$ mm.

Sub-Study (II): Additional Test Cases for Typical Modeling Assumptions

Common atrioventricular heart valve simulation assumptions include prescribing a spatially homogeneous leaflet thickness, and spatially homogeneous leaflet material properties. To test the former assumption, we constructed a synthetic solution containing regionally varying thicknesses in the range [0.1,0.4] mm (**Fig. S6a**) and generated a contour surface (**Fig. S6b**). For the latter assumption, the synthetic solution was constructed by random sampling of material parameter combinations within the ranges $c_1 \in [0.109,0.309]$ kPa and $c_2 \in [10.65,12.65]$ (**Fig. S6c**) and visualized the corresponding errors (**Fig. S6d**). This range was chosen based on our previous biaxial testing study of the regional mechanical properties of the tricuspid valve anterior leaflet where we found minimal spatial variations in the stress-stretch behaviors.

For the case where the synthetic solution contained regionally varying thicknesses, we found the valley of nearly equivalent solutions to shift towards smaller values of c_1 and c_2, however the general shape of the valley was not noticeably different (**Fig. S6b**). This finding suggests that assuming a spatially homogeneous thickness would not significantly affect the inverse finite element analysis. Meanwhile, we observed the opposite trend in the case where the material parameters are heterogeneous: i.e., a more substantial shift of the location of the global minima region towards larger values of c_1 and c_2 (**Fig. S6d**).

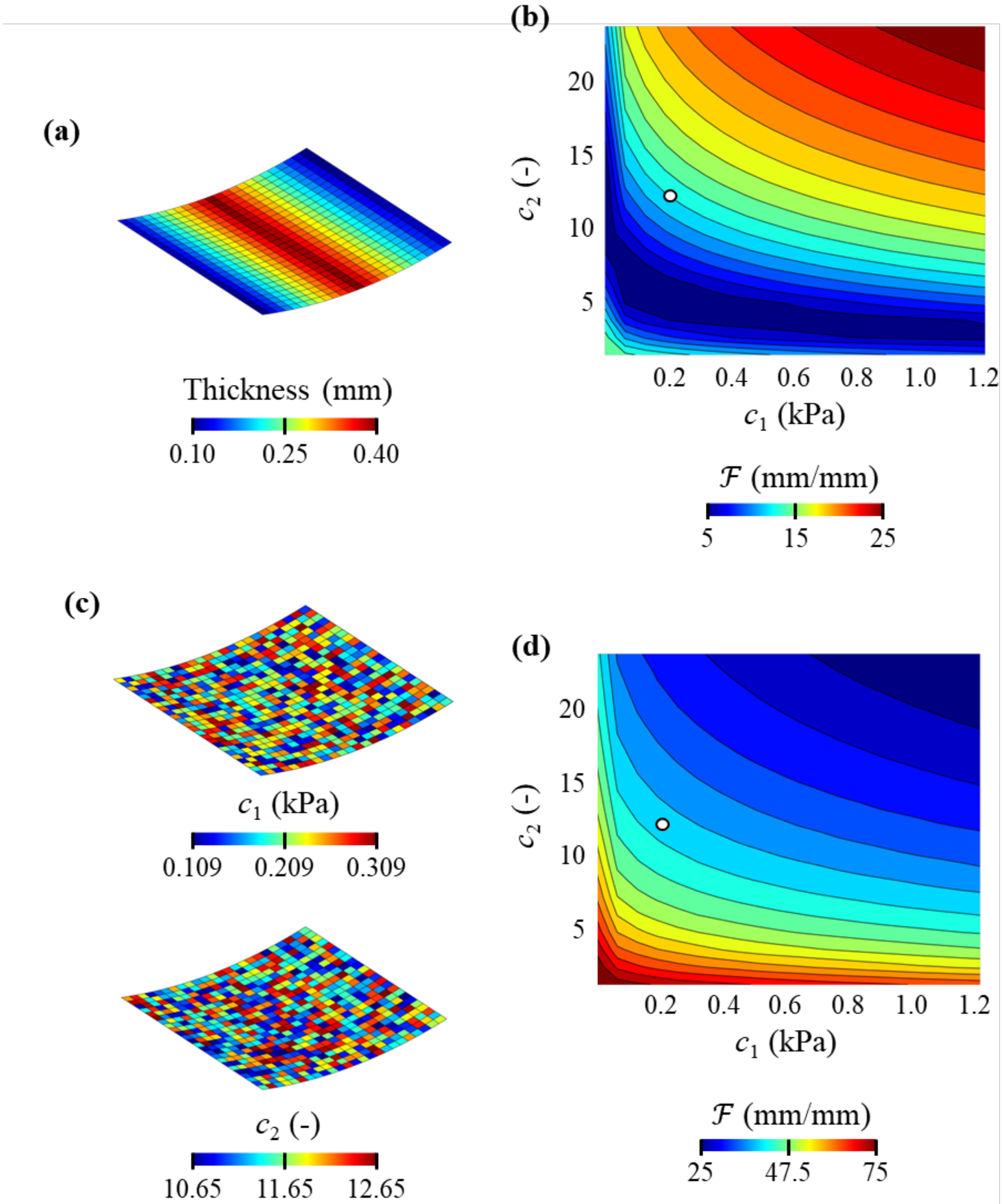

Figure S6: (a) Map of the prescribed regionally varying thicknesses and (b) the corresponding contour surface. (c) Prescribed regionally varying material properties and (d) the corresponding contour surface.