Advancing Nitinol Implant Design and Simulation through Data-driven Methodologies

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Abstract

Recent advances in the Data Science methods for acquiring and analyzing large amounts of materials deformation data have the potential to tremendously benefit Nitinol (Nickel-Titanium shape memory alloy) implant design and simulation. We review some of these data-driven methodologies and provide a perspective on adapting these techniques to Nitinol design and simulation through a three-tiered approach. The methods in the first tier relate to data acquisition. We review methods for acquiring full-field deformation data from implants and methods for quantifying uncertainty in such data. The second tier methods relate to combining data from multiple sources to gain a holistic understanding of complex deformation phenomena such as fatigue. Methods in the third tier relate to making data-driven simulation of the deformation response of Nitinol. A wide adaption of these methods by the cardiovascular implant community may be facilitated by building consensus on best practices and open exchange of computational tools.

Keywords: Nitinol, Shape Memory Alloys, Modeling, Data-driven

1. Introduction

Data Science – a collection of scientific methods to gather and analyze data – has emerged as a versatile tool to advance the descriptive and predictive capabilities in various areas of science and engineering. As an example of the descriptive capabilities, data science enables determining parameters that most influence the response of a system. It also enables quantification of uncertainty in the measurements of the behavior of a system. In terms of the predictive capabilities, data science enables the development of predictive models for the response based on the observed data and not on analytically-derived functions based on a postulated form or ansatz. The tools in this data-driven paradigm such as high-speed and multi-modal data acquisition, efficient data storage and retrieval, and statistics-related learning techniques such as machine learning (ML) have already found several applications specific to the mechanics of structural materials [1, 2]. Cardiovascular implant design that relies on the mechanics of the underlying materials can greatly

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benefit by adapting this data-driven paradigm. Nitinol or Nickel-Titanium shape memory alloy, which is one of the most common materials used in these devices, exhibits monotonic and cyclic mechanical behavior that is complex enough to warrant over four decades of continuous scientific attention. The monotonic mechanical response of Nitinol is challenging to model and predict due to the presence of superelasticity, anisotropy, and strong dependance on the processing parameters [3]. The cyclic response of Nitinol is even more challenging to predict because of the structural and functional fatigue caused by the interaction between the deformation mechanisms of phase transformation and plasticity and the large-cycle regime (10^7-10^9 cycles) relevant to the cardiovascular implants [4, 5]. Because of these complexities, the simulation of Nitinol-based implant deformation typically relies on phenomenological models that rarely account for the specificities of pre-processing and microstructure that affect the mechanical behavior of Nitinol materials used in individual products. The versatile data-driven approach holds the potential to advance the simulation of the deformation behavior of Nitinol. Considering how commonplace computer simulation is in the design of Nitinol-based cardiovascular implants, this advance can positively impact the industry practice.

Since Nitinol deformation simulation is expected to be predictive, it is essential to develop reliable methods to acquire data that will act as inputs to the simulation. In many instances, the availability of input data is limited. Thus, it is advantageous to merge data from multiple available sources. Above all, simulation is one of the available tools when designing Nitinol-based medical devices or when demonstrating durability of such devices under a particular use case. Because of this, it is essential to quantify and communicate the credibility of data used to build the simulations and also quantify the credibility of simulation results. With the knowledge of the simulation credibility, the role played by simulations in a risk-informed decision making scheme can be appropriately determined.

With this motivation, this article reviews the recent advances in the field and provides a perspective on the adaption of the data-driven experimental and modeling methodologies to Nitinol mechanics. Considering that the field is nascent, we propose a three-tiered approach. The tiers are illustrated in Figure 1. The first tier relates to the acquisition of Nitinol material property data and quantification of the uncertainty in the data. This is referred to as the *information* tier. The second tier relates to fusing multi-modal data to reveal mechanisms that fundamentally determine the Nitinol mechanical behavior. This is referred to as the *knowledge* tier. The third tier relates to making performance or property predictions based directly on the available data rather than relying on subjectively-derived analytical expressions or phenomenological models based on a postulated form or ansatz. This is referred to as the *prediction* tier.

Recent advances in the data-based methods related to these three tiers are summarized in the next three sections. We first describe methods in information tier that enable acquisition of Nitinol material deformation data and also enable quantification of the credibility of that data. Then we describe methods in the knowledge tier that facilitate assimilation of data from multiple sources to uncover knowledge about deformation mechanisms. Finally, we review methods in the prediction tier to simulate the deformation

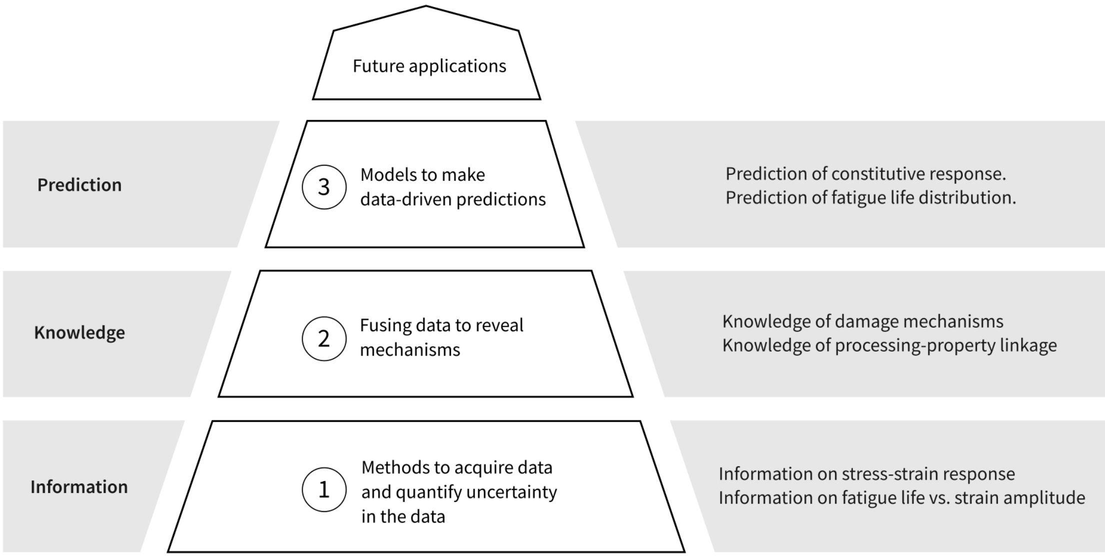

Figure 1: A three tiered approach to incorporating data-driven methods in the modeling of Nitinol mechanics.

of elasto-plastic materials. We provide a perspective to extend these methods to simulate the deformation response of superelastic Nitinol implant components. These methods fundamentally differ from the existing simulation approaches in that they learn the stress-strain relationship or the constitutive law based on any available deformation data and depend less on subjective postulates regarding the form of the constitutive law. We close by summarizing the review and providing a short discussion on promoting a broader adaption of these data-driven methodologies by the Nitinol community.

2. Methods to Acquire Data and Quantify Uncertainty in the Data

Experimental data is used in simulations of Nitinol deformation for various purposes. Most fundamentally, the experimentally measured constitutive response data or the stress-strain curves inform the deformation modes that need to be simulated. Tensile testing data on medical-grade Nitinol inform us that elasticity, superelasticity, and plasticity are three deformation modes through which Nitinol deforms. Experimentally-measured constitutive response data is also used to determine simulation model parameters. This process is typically known as model calibration or material property determination. Finally, experimental data is used to validate the simulation results. For example, the superelastic material properties in many medical device deformation simulations are determined using tensile test data. Then, the simulation results are validated by performing separate simulation of a different deformation mode such as bending or radial loading and comparing the results with corresponding experimental data.

The experimental data acquired for these purposes could either be global or full-field. Global data refers to measurements such as the load measured on a specimen that is tested in tension or the tensile strain averaged over the gage of the specimen. Full-field data on the other hand provides a spatially resolved measure of deformation. Full-field measurements provide a larger quantity of data in a single measurement compared to global measurements. Thus, full-field deformation measurements have become commonplace for informing simulations or for validation of the models.

2.1. Full-field Data Acquisition Methods

Several methods have been demonstrated for measuring the full-field deformation of metals and specifically, the deformation of shape memory alloys [6]. These methods include surface measurement techniques such as digital image correlation (DIC) and Moiré Interferometry and volume measurement techniques such as 3D high-energy X-ray diffraction [7, 8].

The DIC technique for measuring full-field surface strain field has been widely adapted in academic settings [9]. DIC relies on imaging a quasi-random pattern on the surface of the test specimen at certain intervals and analyzing the change in the pattern to calculate surface displacement and strain fields. An important application of DIC to mechanical behavior simulation is in terms of the identification of model parameters including the material properties. Pierron and co-authors provide a detailed overview of various methods for identifying the material properties using DIC measurements [10, 11]. The large amount of data acquired using DIC can help obtain more accurate material properties for complex constitutive models such as those for Nitinol superelasticity. Another application of DIC is in the validation of finite element analysis (FEA) models of deformation [12]. Comparing local deformation results between simulation and DIC measurement can provide a more appropriate validation of the model versus comparing just the global results such as load. While the DIC technique has received wide adaption in the automotive, aerospace, and other industries, it has received relatively small adaption in the medical device design industry.

Aycock and co-authors recently described a detailed framework for measuring full-field deformation on the surface of Nitinol medical devices [13]. They also provided detailed methodology and analysis for quantifying the noise in the acquired data. Acquisition of full-field deformation data from actual medical devices can provide a more effective means of validating computer simulation models used in the design or durability assessment of that particular device. Senol and co-authors have described the use of DIC to validate fatigue strain simulations of a Nitinol test specimen [14]. These approaches can be combined to develop an end-to-end workflow to inform and validate the simulations used in the durability assessment of a Nitinol device. Such a workflow can even provide an experimental substitute to the calculation of fatigue safety factor of a Nitinol implant subjected to particular boundary conditions. An example workflow for the direct evaluation of fatigue indicator parameters and potentially for the evaluation of the fatigue safety factor is shown in Figure 2 and further described in [15]. The workflow first establishes a standard test specimen representative of the geometry of that particular medical device (Figure 2(a)). Here we show a diamond specimen that has historically been used to represent the unit cell of a typical stent. However, the workflow is generic and can be applied to other specimen geometries as well [16, 17] and can be applied to test coupons cut from an actual device. Then, a DIC test setup to measure the surface strains in the specimen is constructed (Figure 2(b)). A variety of commercial DIC setups are available or they can be built using an appropriate selection of cameras, lighting systems, environmental control solutions, and DIC post-processing software. A cyclic loading protocol (Figure 2(c)) to impose a cyclic deformation on the specimen is needed. While the protocol can be as simple as a pre-deformation followed by cyclic application of a displacement range, a protocol that is more representative of the anatomical boundary conditions experienced by the implant can be developed. Using these three pieces of infrastructure, the surface strain fields on the implant can be measured. The surface strain fields can be used to calculate the fatigue strain map or the point cloud of strain amplitude vs. mean strain as shown in Figure 2(d) using an appropriate scalar or tensor method [18]. The data in turn can be used to plot distributions of the mean strain (Figure 2(e)) or the strain amplitude (Figure 2(f)) on the device profile. These data can be subsequently used to determine the fatigue safety factor. While this approach is limited to the fatigue strain assessment on the specimen surface and perhaps one surface of the specimen geometry facing the DIC camera system, it may be adequate since critical fatigue strains often occur on the specimen surface rather than in the interior volume for many common device geometries.

As described in the example above, the DIC technique has tremendous potential utility in the quantification of medical device deformation and in complementing simulation. Continuing advances in the test hardware will make this technique more accessible to the medical device industry. Advances in data science are also leading to advances in the full-field deformation characterization methods. Recently several authors have implemented algorithms for full-field deformation quantification using deep learning, a statistical data analysis method in the family of ML techniques [19, 20]. These techniques provide an alternative to DIC for obtaining surface strain fields. Zhu and co-authors have applied computer vision techniques to obtain surface strains [21]. These advancement mean that full-field data acquisition can be a useful new tool for informing and validating medical device deformation simulations.

2.2. Methods for Uncertainty Quantification

While inputs, methods, and outputs of medical device deformation simulations often receive extensive scrutiny, one aspect that generally receives a lower attention is the uncertainty of the inputs and the consequent credibility of the simulation results. For example, in simulation studies for assessing fatigue safety of medical devices, it is typically seen as adequate to report a fatigue safety factor greater than one. In reality, a fatigue safety factor greater than one means little if the simulation is based on inputs that have a large uncertainty associated with them. Thus, reporting of uncertainty in experimental or simulation data is just as important as acquiring that data.

Recently, various efforts have developed consensus methods of evaluating and communicating credibility

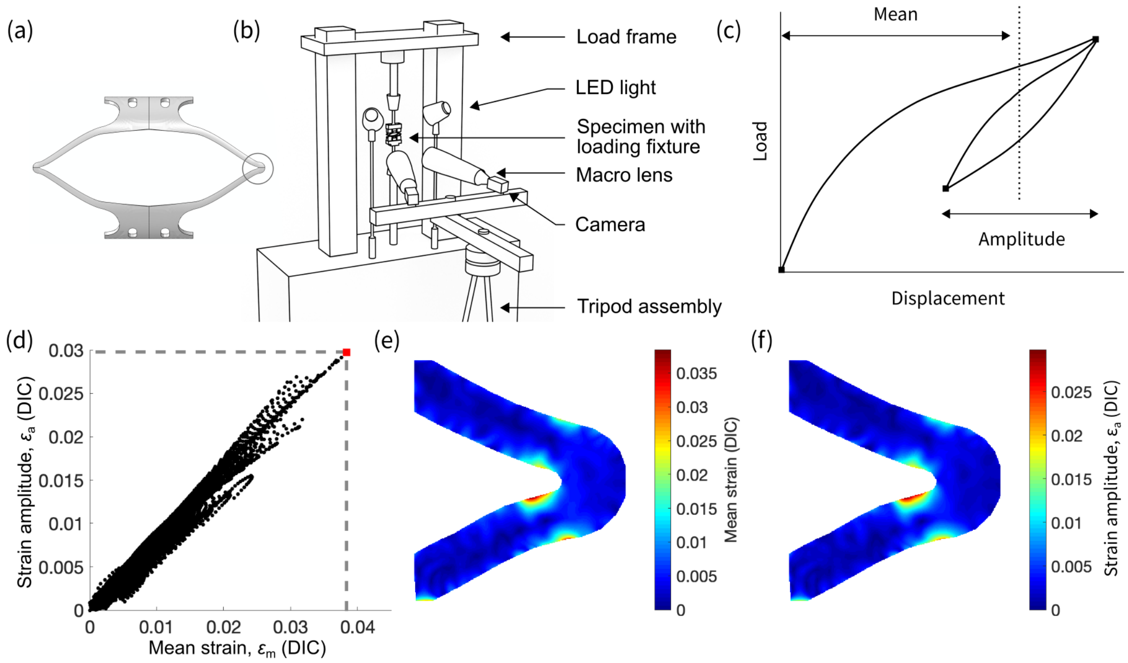

Figure 2: Full-field strain measurement on a diamond Nitinol test specimen during cyclic loading. (a) Schematic of the diamond specimen. (b) Schematic of the digital image correlation (DIC) setup. (c) Schematic of the global load-displacement response showing initial monotonic loading and then cyclic loading in a subcycle. (d) Strain point cloud in the subcycle obtained from full-field surface strains on the diamond measured using digital image correlation. (e) Experimentally measured mean strain distribution in the diamond apex region. (f) Corresponding strain amplitude distribution.

of computational models [22–24]. Overall, they recommend that the credibility of a computational model should be commensurate with the level to which its results are used in making final decisions related to device efficacy or safety. Once an expectation on the credibility of computational model is set, some of the methods reviewed below can be used to assess the uncertainty in the inputs to the computational models and then propagate those input uncertainties to the simulation results.

Ricciardi and co-authors propose a framework for quantifying uncertainties in simulation model parameters when they are determined using experimental data [25]. Their approach is based on Bayesian inferential framework. The Bayesian approach is a statistical method that allows estimation of the probability of a hypothesis being correct based on the available information. This is an appropriate tool for structural mechanics when the intent is to determine the probability distribution of certain mechanical parameters based on available experimental data. The use of Bayesian inference applied to model parameter determination is a well-established practice in structural mechanics [26, 27] and other engineering disciplines [28]. However, until recently, this method has not been applied to the simulation of medical device deformation. Paranjape and co-authors recently applied the technique to determine the probability distribution of superelastic FEA material parameters based on available full-field strain and global load data [29]. They also demonstrated that the uncertainties in the superelastic material parameters can be propagated to the simulations of fatigue safety factor determination. This furnishes a fatigue safety factor value and its credibility intervals. A narrow credibility interval corresponds to a lower uncertainty in the results.

The topic of using probabilistic methods such as the Bayesian method for calibrating the inputs of a constitutive model receives some resistance because of the perception that they incur significantly higher upfront effort compared to the more typical ad-hoc methods. There continues to be development of more efficient methods such as efficient sampling strategies for Bayesian calibration that will continue to reduce this burden [30]. More generally, Cranmer and co-authors list opportunities for advancement for these probabilistic methods in three areas - better determination of uncertainty distribution using smaller input datasets, improving how accurately the uncertainty distribution is determined based on the input model parameters, and making uncertainty quantification more modular such that new data can be sequentially plugged in to update the probability distribution [31].

The statistical methods to quantify the uncertainty in simulation parameters and results are well established and implemented in a variety of common computational tools such as Python and Matlab. As reviewed above, full-field data acquisition methods that can be used to inform such Bayesian inference methods of input parameter determination and uncertainty quantification are also well established. Thus, we are in a position to broadly adapt these methods and make input and output uncertainty quantification a standard practice in the simulation of Nitinol medical device deformation. The methods described here can also be applied to other simulation inputs such as anatomical boundary conditions that are determined from computed tomography, radiography, or other experimental means.

The methods described in this section were in the information tier of the three-tiered approach for adapting data-driven methods to Nitinol implant design and simulation. The knowledge tier methods described below to uncover patterns and mechanisms for deformation phenomena such as fatigue benefit from the methods described in this section.

3. Methods to Fuse Data and Uncover Mechanisms

Many mechanistic problems encountered in the design of cardiovascular implants cannot be directly solved by acquiring experimental data using the sophisticated methods described above. Nor they can be solved by sophisticated simulations alone. Modeling of fatigue is one such problem. Fatigue is a loss in functionality, loss in strength, or catastrophic fracture in components due to cyclic loading. Many implantable medical devices are subjected to cyclic loading due to the cardiac rhythm and are prone to fatigue failure. Thus, demonstration of durability is an important step in the design of implants. A key input in determining the durability of an implant is the fatigue resistance of the underlying Nitinol material itself. It is generally accepted that the fatigue resistance characterization of the base material should be performed to an equivalent number of cycles as the actual device is expected to be exposed to [32]. If the implant under consideration is in the structural heart space, this means that the base material might need to be tested to 600 million cycles. Such testing is expensive and time consuming. Instead, if a model is available that can predict the fatigue resistance distribution at a given fatigue life or the fatigue life distribution at a given resistance, it can significantly reduce the amount of testing required. Further, such model can be used to estimate fatigue resistance even if changes to material purity and pre-processing factors such as cold work are made at an intermediate phase during the implant design process. Thus, we first review data-fusion approaches in the literature related to fatigue life prediction of elasto-plastic and superelastic materials and particularly focus on approaches that have used data science tools such ML.

Sangid reviewed opportunities for combining data from multiple sources to more efficiently predict deformation and failure modes of structural materials [33]. A particular opportunity they mention is using microstructural simulations to augment the fatigue data so that fatigue strain-life curves can essentially be extrapolated to lower fracture probabilities. Chen and Liu provide a comprehensive review of ML approaches used in the modeling of various fatigue-related phenomena [34]. In one particular example, Gebhardt et al. combined impurity shape information from micrographs and fatigue strength information from microstructural simulations to develop a model for fatigue life of nodular cast Iron. The impurity size and shape distribution were the inputs to the model. They used a ML tool called simplified ResNet [35]. Specific to Nitinol, Kafka and co-authors, building on the work of Moore et al., developed an approach to predict the fatigue life of Nitinol at a fixed strain amplitude as a function of particle-void-assembly size and location [36, 37]. They combine highly simplified inclusion size data from 3D characterization with a microstructural model for plastic deformation. Inspired by these examples and particularly by the work of Durmaz et al. [38] on prediction of fatigue life based on microstructural data from multiple sources, we now provide a perspective on an approach to predict the fatigue life of Nitinol based on microstructural information.

An example approach based on data fusion that can be used to predict fatigue life or fatigue resistance of Nitinol base materials is illustrated in Figure 3. The goal of this approach is to predict the fatigue life distribution or fatigue strength distribution of a Nitinol base material when information on the impurity or non-metallic inclusion shape and size distribution is known. By *Nitinol base material* we mean sheet, strip, tubing or similar Nitinol material forms that have undergone a particular processing sequence. By *fatigue life* we mean the number of cycles required to cause fracture at a given strain amplitude. By *fatigue resistance* we mean the strain amplitude requited to cause fracture at a given number of cycles. By *distribution* we mean a median value and associated uncertainty bounds or an equivalent uncertainty quantification. The proposed approach will be developed in three phases. The three phases schematically shown in Figure 3 are described below.

The first phase, named the *test method design* phase, involves selection of Nitinol materials of various microstructural attributes and the design of a test specimen that can be used to make a fatigue test coupon.

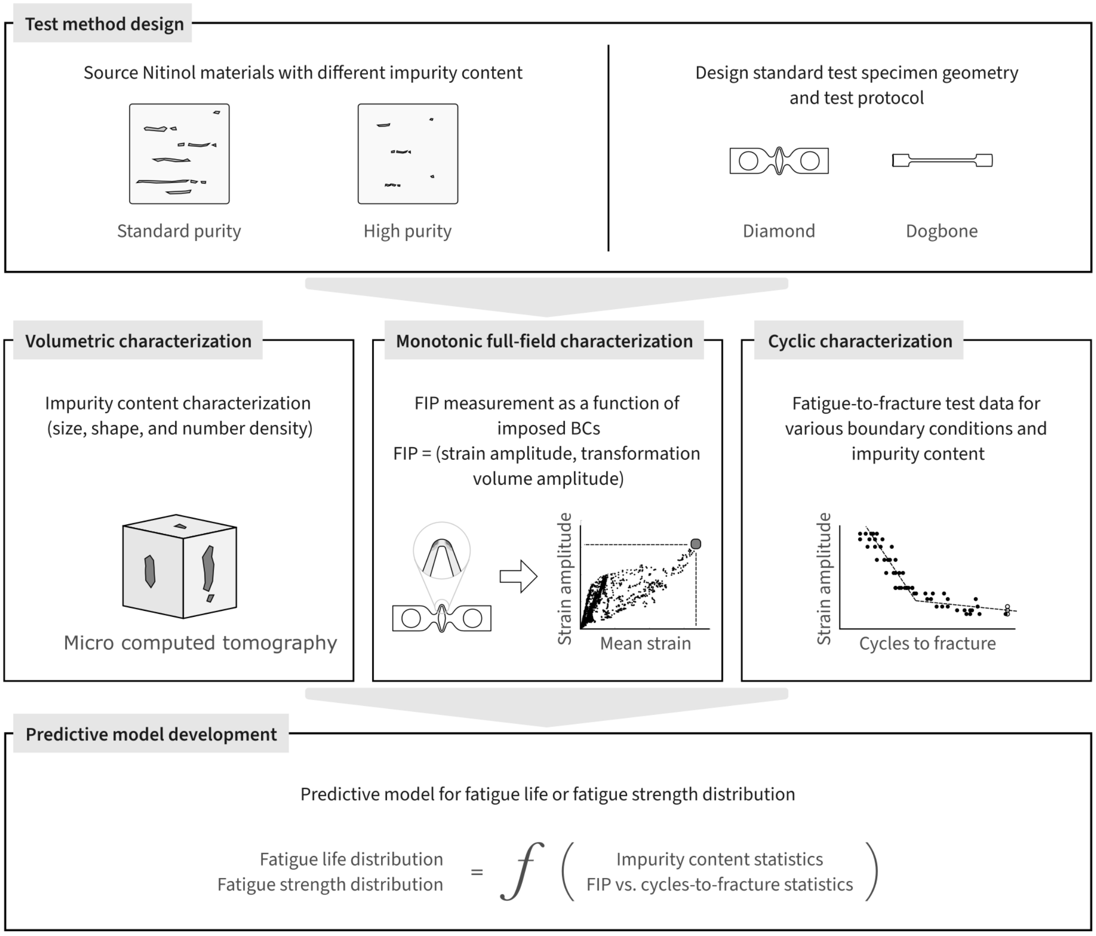

Figure 3: An example of a data fusion strategy for developing a predictive model for fatigue life or fatigue resistance of a Nitinol base material. FIP standard for fatigue indicator parameter.

This may include materials with differing Oxygen and Carbon content, particle-void-assembly area fraction, inclusion morphology distribution, and cold work. Diamond, dogbone, and C-shaped dogbone [16] are some of the specimen geometries that may be considered for making the test specimens from these materials.

The second phase – the *characterization* phase – involves a multi-modal characterization of the microstructure and the fatigue performance of these materials. The microstructural attributes that most significantly influence the fatigue performance will be selected. This selection can be performed using statistical methods such as principal component analysis or it can be informed by data in the literature regarding property-fatigue performance correlation. Significant work on identifying key microstructural parameters influencing fatigue has been performed on Ti-based alloy systems [39, 40] and it can be extended to Nitinol. These microstructural attributes will be characterized in the Nitinol materials using 2D and 3D methods. 2D characterization methods include metallography and scanning electron microscopy to identify non-metallic inclusion fraction. 3D methods include micro-computed tomography that provide volumetric information on the microstructural elements. A full 3D characterization of the microstructural elements may be more desirable because of the anisotropy inherent to most drawn Nitinol products. A monotonic and cyclic performance characterization will be performed on the test specimens manufactured from these materials using displacement boundary conditions that result in a range of mean strains and strain amplitudes that typically occur in cardiovascular implants. The monotonic characterization will be performed to determine the relation between displacement boundary conditions and strains. While this function is typically performed using simulation methods such as FEA, a fully experimental approach using methods such as DIC, as described in Figure 2 may be advantageous. Cyclic characterization will be performed under these displacement boundary conditions to obtain fatigue-to-fracture data. These data can be later used to determine fatigue resistance for a specific fatigue indicator parameter (e.g., strain amplitude). Fatigue-to-fracture data allows calculation of the fatigue strength distribution or fatigue life distribution. The testing will be performed to a reasonable number of cycles representative of the clinical area where these models will be eventually used. For example, if the fatigue data will be used for Nitinol heart valve design, then tests to 600 million cycles should be performed. If the data will be used for the design of peripheral vascular prostheses, then tests to 100 million cycles could be performed. The monotonic and cyclic characterization together provides a map of the fatigue resistance of the material as a function of mean strain and strain amplitude or other similar fatigue indicator parameters.

In the third phase, referred to as the *modeling* phase, a model for fatigue resistance and fatigue life will be constructed. The fatigue resistance and fatigue life will be modeled to be a function of the microstructural parameters such as impurity size and a function of the fatigue indicator parameters such as mean strain and strain amplitude. Relatively simple regression methods can be used to construct the model. However, recently, ML and other statistical methods have made several other tools available for such model construction [34]. Many prior works in the literature related to fatigue life model generation have focussed on the stress-life models. However, the methodologies documented in those works can be extended to strain-life approach relevant to Nitinol. Barbosa and co-authors described a ML method to fit stress-life models to mean stress, stress amplitude, geometric parameters, and fatigue life data [41]. Chen and Liu developed an ML model for determining fatigue life as a function of multiple inputs [42]. Their model is able to incorporate mechanistic constraints based on common observations related to the fatigue life vs. mean stress relationship. Their model is also able to incorporate both fracture and runout data. Statistical methods other than ML can also be used to develop models of fatigue life. Dourado et al. developed a Bayesian fitting method for strain life data [43]. Their method enables the quantification of uncertainty in the fatigue life predictions performed using the model. Whichever is the method used to construct the model, the utility of this data-based approach is that the fatigue life or fatigue resistance of materials that have not been tested before can be predicted using this data-driven framework. The fatigue model development described here may also be able to uncover new dependencies between fatigue life and various processing parameters or microstructural parameters.

The methods in the knowledge tier, described in this section, are primarily descriptive and in part predictive. We now provide a review and perspective on predictive data science methods for Nitinol design and simulation.

4. Methods to Make Data-driven Predictions of Nitinol Deformation Response

The most impactful utility of data-driven methods is in terms of their predictive capabilities. The ability to predict the deformation response of a Nitinol component under various boundary conditions on the basis of a limited information on the constitutive response of the base material is essential in the design of Nitinol implants. Various constitutive modeling and simulation tools such as FEA typically provide this capability. Constitutive response of a material is the relation between stress and strain. Knowledge of accurate constitutive response is one of the most important prerequisites for reliable simulation of Nitinol implant deformation. While the implementation of the constitutive response of Nitinol in simulation tools has incrementally advanced over the years, a leap in the realistic constitutive modeling can significantly enhance the accuracy of simulation of implants. It will also contribute to making in-silico evidence of device durability a widely accepted part of the device regulatory approval process. A field where data science methods are used to develop simulation methods for the constitutive response has emerged. These methods are often referred to as data-driven constitutive modeling. Several methods have been proposed for the data-driven simulation of elasto-plastic deformation. If applied to the superelastic deformation simulation, these methods can significantly advance the simulation of Nitinol deformation.

Data-driven methods of constitutive response simulation can be broadly grouped in two closely-related categories: Surrogate models and model-free data-driven methods [44]. Surrogate models use stress-strain data from existing state-of-the-art simulation methods and create a computationally efficient surrogate regression model using methods such as deep neural networks. Regression-methods-based surrogate models can be efficient because they do not need to iteratively solve the field evolution equations in order to determine the local load or stress response. Model-free data-driven methods on the other hand train the constitutive response based on indirect data. For example, they derive the stress-strain response at a material point based on an experimental dataset consisting of global load and local surface strain histories. This derivation of the constitutive response is generally performed under the constraint of applicable physical laws such as equilibrium and conservation of energy. The model-free methods are notable such that they directly derive the deformation mechanics from the experimental data and do not rely on expert judgement or local stress-strain history from a pre-built higher-fidelity simulation data library to define a particular model form.

Development of surrogate models for history-dependent constitutive response such as elasto-plastic response has been explored for several decades [45]. However, it has become feasible in the last few years due to the increased availability of computational resources and the availability of easy-to-use implementations of sequence learning methods such as long short term memory (LSTM) and gated recurrent units (GRU). Work of Mozaffer et al. was one of the first studies to develop a surrogate model for path-dependent plastic deformation response in 2D [46]. They used a simulation library as an input and used the GRU sequence-learning ML method. Their method is able to capture material hardening and stress concentration due to local inhomogeneities. Other similar approaches have demonstrated enhanced capabilities such as modeling of constitutive response with anisotropic yield behavior [47], using temporal convolutional network (TCN) – another ML sequence learning technique – to provide a surrogate for visoplastic and temperature-dependent response [48], using Linearized Minimal State Cell – a form of recurrent neural network – to obtain a data-driven plasticity surrogate model from long sequences of stress-strain history data [49], and the use of internal state variables [50]. Liu et al. present another innovation in developing a surrogate model for plasticity based on the simulation data obtained at a finer length scale [51]. That is, they train a data-driven surrogate model on the stress-strain data obtained using finer-length scale simulations that implement constitutive modeling techniques such as crystal plasticity and then train a surrogate model form component-level simulations that yield macro-scale stress as a function of a macro-scale strain increment. The work of Karapiperis et al. is in the same domain as it seeks to build a data-driven constitutive law based on lower length-scale simulation results [52].

The model-free data-driven methods of simulation for inelastic materials have been developed in the last few years. Eggersmann and co-authors developed a data-based approach to build a constitutive law [53]. While their approach fundamentally depends on the availability of local stress-strain data pairs to train the constitutive law, their collaborators have demonstrated methods that can extract the requisite local stress-strain data from the macro-scale boundary conditions and local strain fields [54, 55]. Moreover these approaches provide options to incorporate internal variables or history variables in the constitutive law determination. The recent work of Langlois et al. provides an extension of this approach where the constitutive law is obtained from an initial approximation of the local stress state [56]. The approximate local stress state is obtained from the local strain field using the finite element model updating (FEMU) method. The local strain field can be measured using methods such has DIC. Huang and co-authors propose a method for building a data-driven history-dependent inelastic constitutive law where they suggest obtaining the stress-strain sequence data for training from experiments on specialized specimens such as biaxial cruciform geometry [57]. Ibañez et al. [58] propose an approach they term as “manifold learning” to determine the inelastic constitutive law. Again, this approach requires stress-strain inputs for training which can be determined using approaches such as those proposed by Cameron and Tasan [59]. Flaschel et al. propose an approach that obtains a constitutive law with an ansatz selected from a catalogue of pre-defined functions [60, 61]. With a reasonably large pre-built catalogue, this approach can be suitable for model any complex stress-strain response.

Each method in this broad collection of data-driven methods has sought to address specific nuances of constitutive law development. Yet all of these methods rely on certain non-trivial statistical techniques such as minimization or ML-based regression to obtain the constitutive law. Thus, these methods tend to be critiqued on two common aspects. First, there are concerns that the *black-box* statistical formulations used in many of these techniques make it challenging to check for any violations of the fundamental thermodynamics or statics principles. This is particularly critical when the data used for training the constitutive law is noisy and contains outliers, which if taken at their face value can lead to non-physical deformation modes. Some efforts such as the work of Masi et al. have attempted to address this concern by encoding the fundamental thermodynamic conservation principles in the structure of the constitutive modeling ML framework itself [62]. This approach is part of a broader effort to develop physics-informed ML methods for various physics and mechanics problems [63]. Second, there are concerns that the large amount of data used to train the constitutive laws using these methods makes it challenging to quantify the uncertainty in the predictions from these models. Thus, there have been attempts to quantify the uncertainty in the ML-based constitutive modeling including the work of Sun et al. [64]. Moreover, researchers such as Koeppe et al. have developed approaches that can develop interpretable models that can be used to describe the mechanics rather than just develop statistically accurate models for constitutive response [65]. All advances reviewed here may seem like at the cutting-edge where only proof-of-concept implementations suitable for simulating very basic boundary value problems are available. While that may be true for many publications listed here, a variety of efforts have demonstrated end-to-end implementations of their approach including incorporation of the data-driven methods in FEA solvers [66, 67].

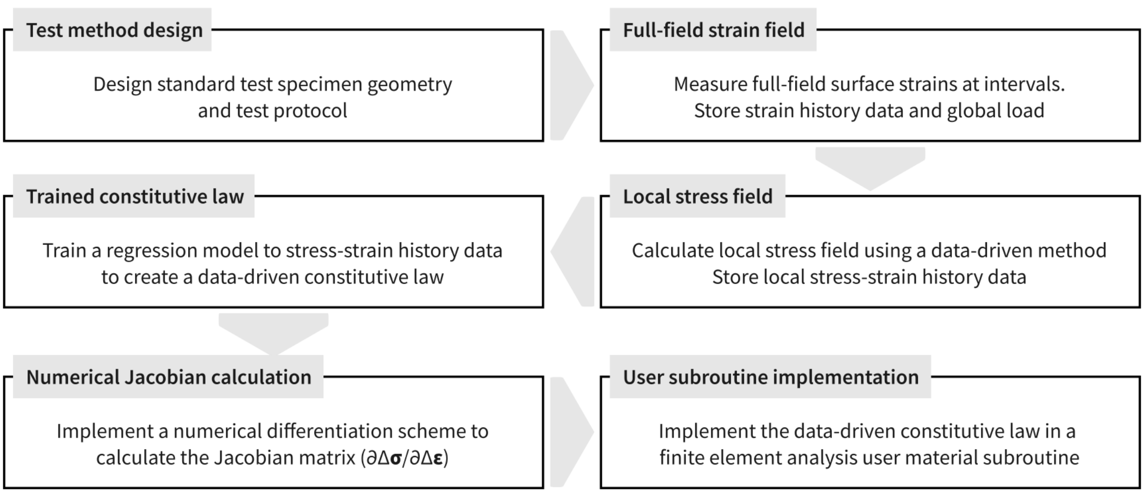

Figure 4: A proposed workflow for developing a data-driven constitutive law for Nitinol superelasticity.

This development of data-driven model-free methods to simulate constitutive response is impressive and we believe we have all the components necessary to develop a data-driven constitutive modeling solution for Nitinol. Such an approach will allow simulation of Nitinol implant deformation based on experimental data obtained from a Nitinol base material that has undergone specific pre-processing. We propose a framework for developing such a simulation method. The framework is schematically shown in Figure 4. It consists of six steps.

1. The implementation begins with the creation of a standard test specimen and test protocol for acquiring experimental data used to train a data-driven constitutive law. The test specimens could be as simple as dogbone-shaped or consist of more complex forms such as cruciform or planar specimens with holes. The specimens should be suitable for acquiring spatial strain distribution history using methods such as DIC.
2. Using the standard test method described above, mechanical testing data under various conditions will be gathered. The test conditions should encompass the conditions that the implant to be modeled will be typically experiencing. The mechanical data could be local strain and global load histories.
3. The implementation then extracts the local stress field from the mechanical data recorded above. This can be achieved using the approach of Stainier et al. [54] or Cameron and Tasan [59] described above. The local stress-strain histories obtained in this step will be stored in a database and will serve as the training and validation data.
4. In this step, a data-driven model will be constructed for the constitutive response using the stress-strain history data described above and a suitable statistical method such as an ML regression scheme. The output of this step is a database of ML regression model hyperparameters that can be stored.
5. FEA implementations of constitutive modeling typically require a constitutive law and a tangent modulus or the Jacobian matrix $(\partial\boldsymbol{\sigma}/\partial\boldsymbol{\epsilon})$ to perform the computation in a discretized implicit time-integration scheme. The Jacobian will be constructed using a suitable automatic numerical differentiation method [67].
6. Once the data-driven constitutive law and the Jacobian are available, they can be programmed in an FEA framework such as the `UMAT` user material subroutine functionality in Abaqus FEA framework.

5. Discussion and Summary

Data science has emerged as a multifaceted tool that can be used to advance various aspects of Nitinol implant design and simulation. We reviewed some of the recent advances in the field and provided a perspective on adapting this tool for various scenarios such as cardiovascular implant deformation characterization, durability prediction, and constitutive modeling. This paradigm shift to data-driven methods is radical and it can be facilitated by adapting a tiered approach. We propose a three-tier approach:

1. Information tier methods for acquiring data on the deformation of implants and methods for quantifying uncertainty in the data. The purpose of these methods is to collect data to be used in the approaches in the two tiers below. The emphasis on uncertainty quantification is to make sure that the credibility information becomes an integral part of any data-driven method development.
2. Knowledge tier methods to enable fusion of data from multiple sources to develop descriptive and predictive models for phenomena such as fatigue. Typically the data is combined from multiple experimental methods such as microstructural characterization, tensile testing, and fatigue testing or from experimental and simulation methods. It is common to analyze a specific aspect of a deformation phenomenon in a reductionist sense using data from a single experimental method. The purpose of methods in this tier is to combine or augment data to promote a holistic analysis of the deformation phenomenon.
3. Prediction tier methods to develop data-driven models for stress-strain response of Nitinol implants. These methods rely on data acquired and assimilated using methods in the information and knowledge tier and sequence-learning methods collectively known as machine learning or deep learning. The purpose of these methods is to increase the speed and accuracy of Nitinol deformation simulation.

The actual adaption of these methods will require the collective effort of the community. Consensus-building will be useful in encouraging participation in this effort. The key concepts, new outcomes, and best practices in these data-driven methods can be discussed at conferences such as the Shape Memory and Superelastic Technologies Conference (SMST), the Cardiovascular Implant Durability Conference (CVID), and the ASTM Committee Weeks to develop community-wide awareness and to promote discussion. The methods can be discussed in working groups modeled after efforts such as Best Practices for Fatigue Assessment of Heart Valve Devices organized by the Heart Valve Collaboratory and consensus best practices may be published. Some of these methods can be standardized through collaboratively developed ASTM standards. The industry participation will also be encouraged if additional research demonstrating proof-of-concept implementation of some of these methods for Nitinol becomes available. These methods inherently depend on customized software tools. Publication of such data science software in open source repositories will reduce duplication of effort across various stakeholders and reduce the overall effort required to adapt these tools. With broad collaboration between various stakeholders, we hope these data-based methods mature quickly and play a central role in the design and simulation of Nitinol cardiovascular implants.

Acknowledgments

HMP would like to thank Confluent Medical Technologies, Inc. for providing the resources for this work.

References

[1] T. D. Sparks, S. K. Kauwe, M. E. Parry, A. M. Tehrani, J. Brgoch, Machine Learning for Structural Materials, Annual Review of Materials Research 50 (2020) 27–48.

[2] R. Arróyave, D. L. McDowell, Systems Approaches to Materials Design: Past, Present, and Future, Annual Review of Materials Research 49 (2019) 103–126.

[3] K. Otsuka, X. Ren, Physical metallurgy of Ti–Ni-based shape memory alloys, Progress in Materials Science 50 (2005) 511–678.

[4] G. Eggeler, E. Hornbogen, A. Yawny, A. Heckmann, M. Wagner, Structural and functional fatigue of NiTi shape memory alloys, Materials Science and Engineering: A 378 (2004) 24–33.

[5] S. W. Robertson, A. R. Pelton, R. O. Ritchie, Mechanical fatigue and fracture of Nitinol, International Materials Reviews 57 (2012) 1–37.

[6] D. Delpueyo, A. Jury, X. Balandraud, M. Grédiac, Applying Full-Field Measurement Techniques for the Thermomechanical Characterization of Shape Memory Alloys: A Review and Classification, Shape Memory and Superelasticity 7 (2021) 462–490.

[7] H. M. Paranjape, P. P. Paul, H. Sharma, P. Kenesei, J.-S. Park, T. Duerig, L. C. Brinson, A. P. Stebner, Influences of granular constraints and surface effects on the heterogeneity of elastic, superelastic, and plastic responses of polycrystalline shape memory alloys, Journal of the Mechanics and Physics of Solids 102 (2017) 46–66.

[8] P. Sedmák, J. Pilch, L. Heller, J. Kopeček, J. Wright, P. Sedlák, M. Frost, P. Šittner, Grain-resolved analysis of localized deformation in nickel-titanium wire under tensile load, Science 353 (2016) 559–562.

[9] B. Pan, Digital image correlation for surface deformation measurement: historical developments, recent advances and future goals, Measurement Science and Technology 29 (2018) 082001. Publisher: IOP Publishing.

[10] S. Avril, M. Bonnet, A.-S. Bretelle, M. Grédiac, F. Hild, P. Ienny, F. Latourte, D. Lemosse, S. Pagano, E. Pagnacco, F. Pierron, Overview of Identification Methods of Mechanical Parameters Based on Full-field Measurements, Experimental Mechanics 48 (2008) 381.

[11] F. Pierron, M. Grédiac, Towards Material Testing 2.0. A review of test design for identification of constitutive parameters from full-field measurements, Strain 57 (2021) e12370. _eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/str.12370.

[12] P. Lava, E. M. C. Jones, L. Wittevrongel, F. Pierron, Validation of finite-element models using full-field experimental data: Levelling finite-element analysis data through a digital image correlation engine, Strain 56 (2020) e12350. _eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/str.12350.

[13] K. I. Aycock, J. D. Weaver, H. M. Paranjape, K. Senthilnathan, C. Bonsignore, B. A. Craven, Full-field microscale strain measurements of a nitinol medical device using digital image correlation, Journal of the Mechanical Behavior of Biomedical Materials (2020) 104221.

[14] K. Senol, H. Cao, S. Tripathy, Characterization and Validation of Fatigue Strains for Superelastic Nitinol Using Digital Image Correlation, Journal of Medical Devices 15 (2021).

[15] J. Angela, D. C. Pagan, J. Gilbert, L. Vien, I. Ong, C. Bonsignore, H. M. Paranjape, A Digital Image Correlation Methodology for the Characterization of Cyclic Deformation in Nickel-Titanium Medical Device Fatigue Test Specimens., Unpublished (2020).

[16] S. Tripathy, M. Wu, H. Cao, Finite Element Framework for Fatigue Performance Assessment of Superelastic Nitinol Used in Medical Devices, in: M. R. Mitchell, B. T. Berg, T. O. Woods, K. L. Jerina (Eds.), Fourth Symposium on Fatigue and Fracture of Metallic Medical Materials and Devices, ASTM International, 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428-2959, 2019, pp. 31–53. URL: `https://www.astm.org/doiLink.cgi?STP161620180039`. doi:`10.1520/STP161620180039`.

[17] H. Cao, M. H. Wu, F. Zhou, R. M. McMeeking, R. O. Ritchie, The influence of mean strain on the high-cycle fatigue of Nitinol with application to medical devices, Journal of the Mechanics and Physics of Solids 143 (2020) 104057.

[18] R. Marrey, B. Baillargeon, M. L. Dreher, J. D. Weaver, S. Nagaraja, N. Rebelo, X.-Y. Gong, Validating Fatigue Safety Factor Calculation Methods for Cardiovascular Stents, Journal of Biomechanical Engineering 140 (2018) 061001.

[19] S. Boukhtache, K. Abdelouahab, F. Berry, B. Blaysat, M. Grédiac, F. Sur, When Deep Learning Meets Digital Image Correlation, Optics and Lasers in Engineering 136 (2021) 106308.

[20] R. Yang, Y. Li, D. Zeng, P. Guo, Deep DIC: Deep learning-based digital image correlation for end-to-end displacement and strain measurement, Journal of Materials Processing Technology 302 (2022) 117474.

[21] C. Zhu, H. Wang, K. Kaufmann, K. S. Vecchio, A computer vision approach to study surface deformation of materials, Measurement Science and Technology 31 (2020) 055602. Publisher: IOP Publishing.

[22] C. J. Freitas, Standards and Methods for Verification, Validation, and Uncertainty Assessments in Modeling and Simulation, Journal of Verification, Validation and Uncertainty Quantification 5 (2020) 021001.

[23] ASME, Assessing Credibility of Computational Modeling Through Verification and Validation: Application to Medical Devices, Technical Report, 2018.

[24] T. M. S. (TMS), Accelerating the Broad Implementation of Verification & Validation in Computational Models of the Mechanics of Materials and Structures, Technical Report 978-0-578-75450-5, The Materials Society, 2020.

[25] D. E. Ricciardi, O. A. Chkrebtii, S. R. Niezgoda, Uncertainty Quantification for Parameter Estimation and Response Prediction: Generalizing the Random Effects Bayesian Inferential Framework to Account for Material and Experimental Variability, Integrating Materials and Manufacturing Innovation 8 (2019) 273–293.

[26] M. C. Kennedy, A. O'Hagan, Bayesian calibration of computer models, Journal of the Royal Statistical Society: Series B (Statistical Methodology) 63 (2001) 425–464.

[27] H. Rappel, L. A. A. Beex, J. S. Hale, L. Noels, S. P. A. Bordas, A Tutorial on Bayesian Inference to Identify Material Parameters in Solid Mechanics, Archives of Computational Methods in Engineering 27 (2020) 361–385.

[28] F. A. C. Viana, A. K. Subramaniyan, A Survey of Bayesian Calibration and Physics-informed Neural Networks in Scientific Modeling, Archives of Computational Methods in Engineering 28 (2021) 3801–3830.

[29] H. M. Paranjape, K. I. Aycock, C. Bonsignore, J. D. Weaver, B. A. Craven, T. W. Duerig, A probabilistic approach with built-in uncertainty quantification for the calibration of a superelastic constitutive model from full-field strain data, Computational Materials Science 192 (2021) 110357.

[30] A. Lye, A. Cicirello, E. Patelli, Sampling methods for solving Bayesian model updating problems: A tutorial, Mechanical Systems and Signal Processing 159 (2021) 107760.

[31] K. Cranmer, J. Brehmer, G. Louppe, The frontier of simulation-based inference, Proceedings of the National Academy of Sciences (2020) 201912789.

[32] {International Standards Organization}, Cardiovascular implants - Cardiac valve prostheses - Part 1: General requirements (ISO 5840-1:2021), 2021. URL: `https://www.iso.org/obp/ui/#!iso:std:77033:en`.

[33] M. D. Sangid, Coupling in situ experiments and modeling – Opportunities for data fusion, machine learning, and discovery of emergent behavior, Current Opinion in Solid State and Materials Science 24 (2020) 100797.

[34] J. Chen, Y. Liu, Fatigue modeling using neural networks: A comprehensive review, Fatigue & Fracture of Engineering Materials & Structures 45 (2022) 945–979. _eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/ffe.13640.

[35] C. Gebhardt, T. Trimborn, F. Weber, A. Bezold, C. Broeckmann, M. Herty, Simplified ResNet approach for data driven prediction of microstructure-fatigue relationship, Mechanics of Materials 151 (2020) 103625.

[36] O. L. Kafka, C. Yu, M. Shakoor, Z. Liu, G. J. Wagner, W. K. Liu, Data-Driven Mechanistic Modeling of Influence of Microstructure on High-Cycle Fatigue Life of Nickel Titanium, JOM 70 (2018) 1154–1158.

[37] J. A. Moore, D. Frankel, R. Prasannavenkatesan, A. G. Domel, G. B. Olson, W. K. Liu, A crystal plasticity-based study

of the relationship between microstructure and ultra-high-cycle fatigue life in nickel titanium alloys, International Journal of Fatigue 91 (2016) 183–194.

[38] A. R. Durmaz, N. Hadzic, T. Straub, C. Eberl, P. Gumbsch, Efficient Experimental and Data-Centered Workflow for Microstructure-Based Fatigue Data, Experimental Mechanics 61 (2021) 1489–1502.

[39] M. W. Priddy, N. H. Paulson, S. R. Kalidindi, D. L. McDowell, Strategies for rapid parametric assessment of microstructure-sensitive fatigue for HCP polycrystals, International Journal of Fatigue 104 (2017) 231–242.

[40] N. H. Paulson, M. W. Priddy, D. L. McDowell, S. R. Kalidindi, Data-driven reduced-order models for rank-ordering the high cycle fatigue performance of polycrystalline microstructures, Materials & Design 154 (2018) 170–183.

[41] J. F. Barbosa, J. A. F. O. Correia, R. C. S. F. Júnior, A. M. P. D. Jesus, Fatigue life prediction of metallic materials considering mean stress effects by means of an artificial neural network, International Journal of Fatigue 135 (2020) 105527.

[42] J. Chen, Y. Liu, Probabilistic physics-guided machine learning for fatigue data analysis, Expert Systems with Applications 168 (2021) 114316.

[43] A. Dourado, F. Irmak, F. A. C. Viana, A. P. Gordon, A Nonstationary Uncertainty Model and Bayesian Calibration of Strain-Life Models, Journal of Verification, Validation and Uncertainty Quantification 6 (2021).

[44] N. Kovachki, B. Liu, X. Sun, H. Zhou, K. Bhattacharya, M. Ortiz, A. Stuart, Multiscale modeling of materials: Computing, data science, uncertainty and goal-oriented optimization, Mechanics of Materials 165 (2022) 104156.

[45] J. Ghaboussi, J. H. Garrett, X. Wu, Knowledge-Based Modeling of Material Behavior with Neural Networks, Journal of Engineering Mechanics 117 (1991) 132–153. Publisher: American Society of Civil Engineers.

[46] M. Mozaffar, R. Bostanabad, W. Chen, K. Ehmann, J. Cao, M. A. Bessa, Deep learning predicts path-dependent plasticity, Proceedings of the National Academy of Sciences 116 (2019) 26414–26420. Publisher: National Academy of Sciences Section: Physical Sciences.

[47] M. B. Gorji, M. Mozaffar, J. N. Heidenreich, J. Cao, D. Mohr, On the potential of recurrent neural networks for modeling path dependent plasticity, Journal of the Mechanics and Physics of Solids 143 (2020) 103972.

[48] D. W. Abueidda, S. Koric, N. A. Sobh, H. Sehitoglu, Deep learning for plasticity and thermo-viscoplasticity, International Journal of Plasticity 136 (2021) 102852.

[49] C. Bonatti, D. Mohr, On the Importance of Self-consistency in Recurrent Neural Network Models Representing Elasto-plastic Solids, Journal of the Mechanics and Physics of Solids (2021) 104697.

[50] K. Ciftci, K. Hackl, Model-free data-driven simulation of inelastic materials using structured data sets, tangent space information and transition rules, Computational Mechanics (2022).

[51] B. Liu, N. Kovachki, Z. Li, K. Azizzadenesheli, A. Anandkumar, A. M. Stuart, K. Bhattacharya, A learning-based multiscale method and its application to inelastic impact problems, Journal of the Mechanics and Physics of Solids 158 (2022) 104668.

[52] K. Karapiperis, L. Stainier, M. Ortiz, J. E. Andrade, Data-Driven Multiscale Modeling in Mechanics, Journal of the Mechanics and Physics of Solids (2020) 104239.

[53] R. Eggersmann, T. Kirchdoerfer, S. Reese, L. Stainier, M. Ortiz, Model-Free Data-Driven inelasticity, Computer Methods in Applied Mechanics and Engineering 350 (2019) 81–99.

[54] L. Stainier, A. Leygue, M. Ortiz, Model-free data-driven methods in mechanics: material data identification and solvers, Computational Mechanics 64 (2019) 381–393.

[55] J. Réthoré, A. Leygue, M. Coret, L. Stainier, E. Verron, Computational measurements of stress fields from digital images: Computational measurements of stress fields from digital images, International Journal for Numerical Methods in Engineering 113 (2018) 1810–1826.

[56] R. Langlois, M. Coret, J. Réthoré, Non-parametric stress field estimation for history-dependent materials: Application to

ductile material exhibiting Piobert–Lüders localization bands, Strain (2022) e12410. Publisher: Wiley Online Library.

[57] D. Huang, J. N. Fuhg, C. Weißenfels, P. Wriggers, A machine learning based plasticity model using proper orthogonal decomposition, Computer Methods in Applied Mechanics and Engineering 365 (2020) 113008.

[58] R. Ibañez, E. Abisset-Chavanne, J. V. Aguado, D. Gonzalez, E. Cueto, F. Chinesta, A Manifold Learning Approach to Data-Driven Computational Elasticity and Inelasticity, Archives of Computational Methods in Engineering 25 (2018) 47–57.

[59] B. C. Cameron, C. C. Tasan, Deterministic calculation of elasto-plastic stress-strain behavior from arbitrary deformation fields, arXiv:2103.11938 [cond-mat] (2021). ArXiv: 2103.11938.

[60] M. Flaschel, S. Kumar, L. De Lorenzis, Discovering plasticity models without stress data, arXiv preprint arXiv:2202.04916 (2022).

[61] M. Flaschel, S. Kumar, L. De Lorenzis, Unsupervised discovery of interpretable hyperelastic constitutive laws, Computer Methods in Applied Mechanics and Engineering 381 (2021) 113852.

[62] F. Masi, I. Stefanou, P. Vannucci, V. Maffi-Berthier, Thermodynamics-based Artificial Neural Networks for constitutive modeling, Journal of the Mechanics and Physics of Solids 147 (2021) 104277.

[63] G. E. Karniadakis, I. G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, L. Yang, Physics-informed machine learning, Nature Reviews Physics 3 (2021) 422–440.

[64] X. Sun, B. Bahmani, N. N. Vlassis, W. Sun, Y. Xu, Data-driven discovery of interpretable causal relations for deep learning material laws with uncertainty propagation, Granular Matter 24 (2021) 1.

[65] A. Koeppe, F. Bamer, M. Selzer, B. Nestler, B. Markert, Explainable Artificial Intelligence for Mechanics: Physics-Explaining Neural Networks for Constitutive Models, Frontiers in Materials 8 (2022) 824958.

[66] D. Liu, H. Yang, K. I. Elkhodary, S. Tang, W. K. Liu, X. Guo, Mechanistically informed data-driven modeling of cyclic plasticity via artificial neural networks, Computer Methods in Applied Mechanics and Engineering 393 (2022) 114766.

[67] D. Z. Huang, K. Xu, C. Farhat, E. Darve, Learning constitutive relations from indirect observations using deep neural networks, Journal of Computational Physics 416 (2020) 109491.