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An introduction to a porous shape memory alloy dynamic data driven application system

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Abstract

Shape Memory Alloys are capable of changing their crystallographic structure due to changes of temperature and/or stress. Our research focuses on three points: (1) Iterative Homogenization of Porous SMAs: Development of a Multiscale Model of porous SMAs utilizing iterative homogenization and based on existing knowledge of constitutive modeling of polycrystalline SMAs. (2) DDDAS: Develop tools to turn on and off the sensors and heating unit(s), to monitor on-line data streams, to change scales based on incoming data, and to control what type of data is generated. The application must have the capability to be run and steered remotely. (3) Modeling and applications of porous SMA: Vibration isolation devices with SMA and porous SMA components for aerospace applications will be analyzed and tested. Numerical tools for modeling porous SMAs with a second viscous phase will be developed.The outcome will be a robust, three-dimensional, multiscale model of porous SMA that can be used in complicated, real-life structural analysis of SMA components using a DDDAS framework.

Keywords: Dynamic Data Driven Application Systems; DDDAS; SMAs; homogenization; modeling; data assimilation

1. Introduction

In this paper we describe an ongoing research project to develop a dynamic data driven application system (DDDAS) for porous Shape Memory Alloys using multiscale methods and finite element methods. A virtual shaker device is described that we use for experimentation in order to determine how many sensors are appropriate, the sampling rate, and how the sensors influence the models.

SMAs can be incorporated in vibration isolation devices since (a) they can sustain large recoverable in elastic strains and dissipate high levels of energy, and (b) can actively tune and damp resonance frequencies. The porous SMA variety (a) has similar macroscopic hysteretic response as their dense counterparts, (b) offers significant

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weight advantages for aerospace applications, and (c) flow of a viscous phase in the pore space can be used for temperature control and additional tuning of vibration isolation characteristics.

In Section 2 we describe Shape Memory Alloys (SMAs). In Section 3 we describe the multiscale model and homogenization. In Section 4 we describe the virtual shaker device and the DDDAS. In Section 5, we provide the conclusion and future work remarks.

2. Shape Memory Allows

Shape Memory Alloys are capable of changing their crystallographic structure due to changes of temper- ature and/or stress. These changes, referred to as martensitic phase transformations, are associated with a transformation from a high symmetry austenitic phase to a low symmetry martensitic phase and vice versa [1]. What makes SMA materials remarkably different from ordinary metals is the shape memory effect and the pseudoelasticity effect which are associated with the specific way the phase transition occurs [2]. The shape memory effect allows material that has been deformed while in the martensitic phase to recover its shape upon heating. The mechanism behind this behavior is the ability of SMAs to allow detwinning of the self-accommodated martensitic variants. The pseudoelasticity in SMAs is their ability to support large inelastic strains recoverable upon unloading due to the reverse phase transformation from martensite into austenite. The primary way in which such strains are introduced in the material is the stress induced phase transformation from austenite into martensite.

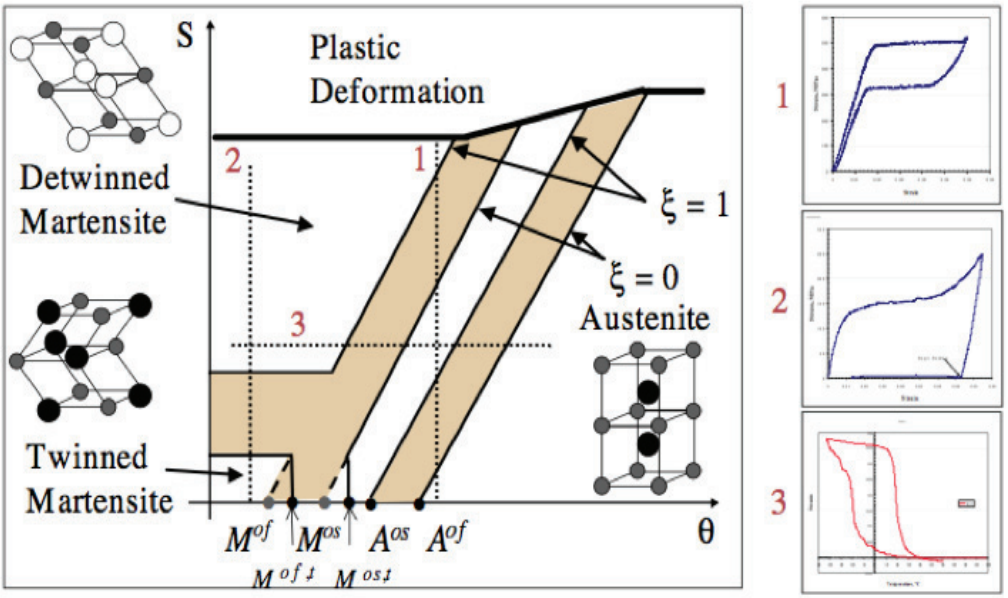

Fig. 1. Stress temperature phase diagram of an SMA

Compared to the other traditional active materials, e.g., piezoelectric and magnetostrictive materials, SMAs show superior performance as high energy density low frequency actuators [3]. Due to their ability to develop large displacements and forces when transformed, SMAs have given rise to their usage in a wide array of applications ranging from orthodontic wires [4] to actuators in robotic systems, self-expanding microstructures [5] and passive vibration isolation devices [6-8] for aerospace applications. A review paper [9] cited many studies on SMA devices used in industries that include mechanical, electronic, automotive, and aerospace.

The analysis of the existing models and their comparison to the experimental results has shown that current SMA constitutive models that take into account the development of stress-induced martensite have reached a high level of sophistication. However, such models generally lack the ability to handle other loading paths involving detwinning

and reorientation of martensite in conjunction with the pseudoelastic response. Therefore, there is need for a 3D constitutive model that can accurately capture not only the material response during pseudoelastic and SME loading paths, but also loading paths that involve co-existence of all the three material phases: austenite, twinned (self-accommodated) martensite, and detwinned martensite. Such a model can be implemented numerically and tested on a comprehensive set of model problems. This lets us perform numerical simulations of problems of varying engineering difficulty, such as the actuation of SMA micro-grips [10], the cooling/heating cycles in the manufacturing and deployment of biomedical devices [11], temperature actuated flow regulating devices [12], and fuel powered SMA actuators [13], just to name a few examples.

We utilize a 3-D constitutive model for polycrystalline Shape Memory Alloys [14]. The model is based on a modified phase transformation diagram that is able to distinguish detwinning from phase transformation behavior. The model takes into account both direct conversion of austenite into detwinned martensite as well as the detwinning of self accommodated martensite (see Fig. 2). It is suitable for performing numerical simulations on SMA materials undergoing complex thermomechanical loading paths in stress-temperature space. The model is based on thermodynamic potentials and utilizes three internal variables to predict the phase transformation and detwinning of martensite in polycrystalline SMAs. The model has been tested extensively on complicated geometries. It can handle complicated thermomechanical loading paths and complex geometries robustly enough so that it can be utilized in an iterative upscaling framework for porous SMAs.

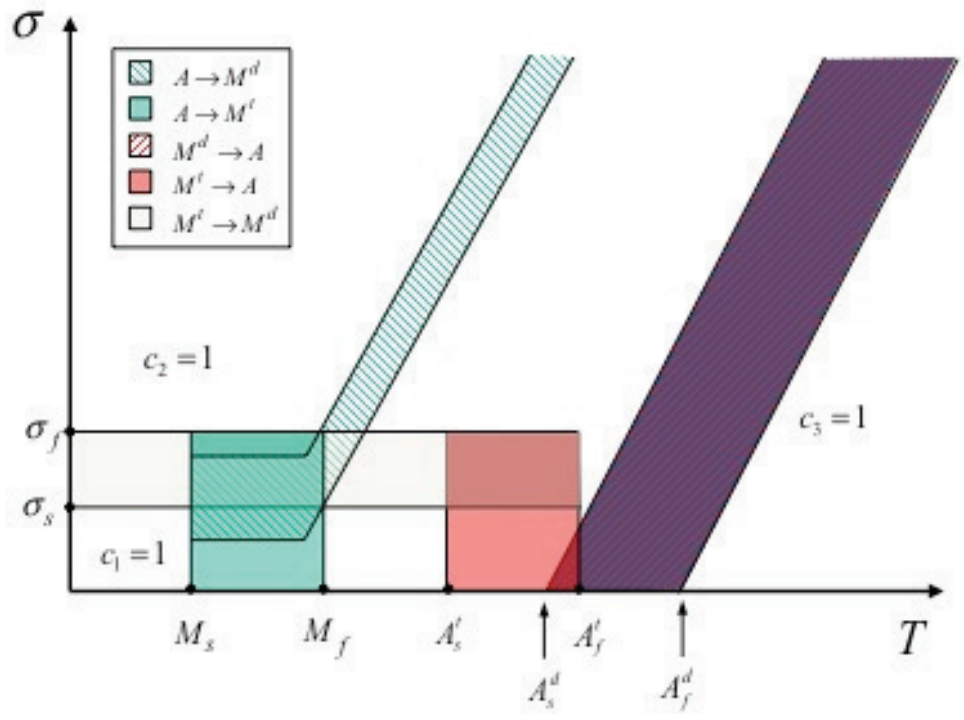

Fig. 2. SMA Phase diagram showing the different transformation regions in stress-temperature space. The diagram is extended in comparisons to previous works in order to achieve a consistent and robust model

The mass fractions of the three phases are introduced:

c_1: self-accommodated martensite
c_2: detwinned martensite
c_3: austenite,

where $c_1+c_2+c_3=1$, $0\le i\le 1$, $i=1,2,3$. The transitions between the different species are accounted by three independent internal variables ξ_1, ξ_2, and ξ_3 that satisfy $c_1=c_{10}+\xi_1-\xi_3$, $c_2=c_{20}+\xi_2+\xi_3$, and $c_3=c_{30}-\xi_1-\xi_2$ (see Fig. 3).

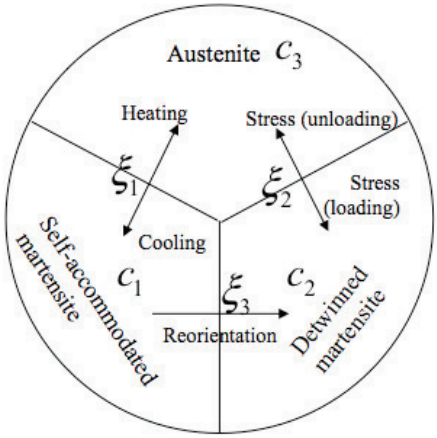

Fig 3. Internal variables for a dense SMA model

We use a general form of the Gibbs free energy for a polycrystalline SMA that at any instance can contain any of three species, σ is the Cauchy stress and T is temperature:

$$G = c_1 G^{(1)}(\sigma,T) + c_2 G^{(2)}(\sigma,T) + c_3 G^{(3)}(\sigma,T) + G^{MIX}(\sigma,T,c_1,c_2,\mu^{in}),$$

where the $G^{(i)}$, $i=1,2,3$ are given by

$$G^{(1)}(\sigma,T) = G^{(2)}(\sigma,T) = -\frac{1}{2\rho}\sigma : S^M : \sigma(1-\frac{1}{\rho}) : \left[\alpha^M (T-T_0)+\varepsilon^{in}\right] + c\left[T-T_0-T\ln(T/T_0)\right] - s_0^M (T-T_0) + u_0^M$$

and

$$G^{(3)}(\sigma,T) = -\frac{1}{2\rho}\sigma : S^A : \sigma(1-\frac{1}{\rho}) : \left[\alpha^A (T-T_0)+\varepsilon^{in}\right] + c\left[T-T_0-T\ln(T/T_0)\right] - s_0^A (T-T_0) + u_0^A$$

Given a set of hardening parameters $\dot{\Omega}_i$, the energy mixing term is given by

$$G^{MIX}(c_1,c_2) = \frac{1}{2}b_1(\dot{\varepsilon}_1)c_1^2 + \frac{1}{2}b_1(\dot{\varepsilon}_2)c_2^2 + b_{12}c_1c_2 + \mathrm{sgn}(\dot{\varepsilon}_1)\mu_1 c_1 + \mathrm{sgn}(\dot{\varepsilon}_2)\mu_2 c_2, \text{ where}$$

$$\beta_i = \beta_i^A \text{ for } \dot{\varepsilon}_i > 0 \text{ and } \beta_i^M \text{ for } \dot{\varepsilon}_i < 0,\ i=1,2.$$

The total inelastic strain ε^{in} is assumed to be generated only by the phase transformation and the detwinning of martensite and is decomposed additively:

$$\varepsilon^{in} = \varepsilon^d + \varepsilon^t, \quad \dot{\varepsilon}^d = \Lambda^d \dot{\xi}_3, \quad \dot{\varepsilon}^t = \Lambda^t \dot{\xi}_2, \quad \Lambda^d = \sqrt{\frac{2}{3}} H \frac{dev(\sigma)}{\|dev(\sigma)\|} \text{ when } \dot{\xi}_3 > 0,$$

$$\Lambda^t = \sqrt{\frac{2}{3}} H \frac{dev(\sigma)}{\|dev(\sigma)\|} \text{ when } \dot{\xi}_2 > 0 \quad \text{and} \quad \Lambda^t = \sqrt{\frac{2}{3}} H \frac{dev(\varepsilon^t)}{\|dev(\varepsilon^t)\|} \text{ when } \dot{\xi}_2 < 0.$$

Here, the tensors Λ^t and Λ^d specify the flow rate for the phase transformation ($A \leftrightarrow M^d$) and the detwinning of the martensite ($M^t \rightarrow M^d$), respectively. The second law of thermodynamics then takes the form

$$T\dot{\eta} = -\left(\varepsilon - \varepsilon^{in} + \rho\frac{\partial G}{\partial \sigma}\right):\dot{\sigma} - \rho\left(s + \rho\frac{\partial G}{\partial T}\right):\dot{T} - \rho\frac{\partial G}{\partial \xi_1}\dot{\xi}_1 + \left(\sigma:\Lambda^t - \rho\frac{\partial G}{\partial \xi_2}\right)\xi_2$$
$$+\left(\sigma:\Lambda^t - \rho\frac{\partial G}{\partial \xi_3}\right)\xi_3 \geq 0.$$

3. Multiscale Modeling and Iterative Homogenization

Over the past few years we have developed a multiscale framework for Fluid-Structure Interaction (FSI) problems that is directly relevant to the proposed research [15]. We consider deformable porous media. Stokes flow is assumed at the pore scale and an elastic model for the pore-level deformations. Because of the complexity of the interaction at the pore level, an iterative macroscopic model is used. The macroscopic model consists of a nonlinear Darcy equation and upscaled elasticity equations. Both constitutive relations are modeled via an iterative procedure. In each iteration, constitutive equations are derived based on macroscopic variables and local cell problems. Numerical results for the case of linear elastic solid skeleton have demonstrated the well-posedness and covnergence of the method. Results show that due to changes in the pore structure, we can substantially increase the permeability of the media. Our numerical studies show a good agreement between the reference solution and the solution obtained from the proposed upscaled model. We have also done analysis under some restrictive assumptions. The main theoretical result is a comparison between the reference fine-scale solution and the downscaled one obtained by iterative upscaling in one macro iteration. In particular, the error at iteration n is estimated, given that the error at iteration $n-1$ is small. Because of the loss of periodicity, partition of unity techniques are employed to construct the correctors for Stokes equations in locally periodic media, which are then utilized in the analysis.

We utilize existing knowledge of constitutive modeling of polycrystalline SMA in order to build a multiscale model based on iterative homogenization, which will span two length-scales: at the fine scale the SMA forms a porous space filled by a fluid, and at the macroscale where the porous SMA skeleton and the fluid are treated as a poroelastic material (Fig. 4). The homogenization is done by iterative upscaling. This is a novel contribution to the field of SMA constitutive modeling, in terms of predicting the macroscopic response of a fluid-SMA mixture.

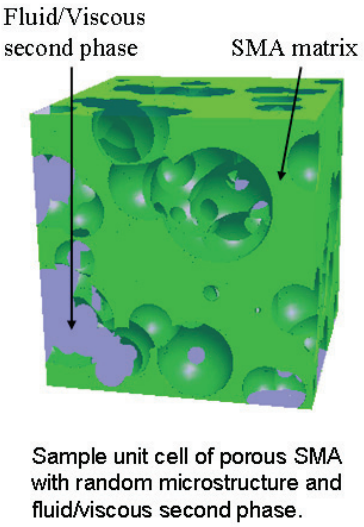

Fig. 4. A schematic of a porous SMA (green) with a fluid second phase (transparent)

We are developing novel multiscale computational models for our applications following the approach in [15]. Our primary tools include ideas from homogenization theory based on iterative homogenization [16-17]. The key idea is to build fine-scale information directly into a coarse scale computational grid, thus bypassing the explicit

homogenization step. This approach allows treatment of problems with highly nonlinear coefficients and/or interface conditions by incorporating the correct fine-scale physics into the coarse level numerically. The main challenge is to adapt those tools to the highly complex and nonlinear nature of the fine scale. When bridging it we have to do uncertainty quantification in ways that ensure that the coarser model retains its predictive capabilities.

The implementation issues associated with numerical upscaling methods are also formidable. They require multiple local solves of a system of nonlinear differential equation in a Representative Element of Volume (REV). This is needed for each nonlinear coarse scale iteration at each coarse grid point. In that step we use the model developed by [14], which has been implemented in a robust way in a displacement based FEM. Moreover, the homogenization step involves random geometries (e.g., the porous skeleton, various material parameters such as maximum transformation strain, etc.). Consequently, iterative homogenization schemes in such stochastic geometries are computationally very expensive. The problem is compounded by the need for nonlinear iterations. On the other hand, homogenization theory allows us to isolate each local problem, leading to a very high degree of parallelism. Hence, numerical upscaling schemes are ideally suited to emerging Petascale computing environments. Such computational resources, either in the form of a massively parallel distributed computer or a cloud architecture, are, in principle, sufficient to treat the model for either application by iterative homogenization. However, we really need entirely new programming concepts as part of this work. These are mandated by the high degree of parallel flexibility required, including the preprocessing of the data at very different scales, the local computational runs themselves, and the post-processing steps. Together with proper uncertainty characterization methods, iterative upscaling on emerging computing architectures has the potential to bridge all the length-scales involved in a robust way and assess the uncertainties in the predictions.

The actual methodology appears straightforward:

- Defines a multiscale mapping linking the coarse fields (displacement, stress, internal variables) to the fine scale quantities (e.g. homogenization motivated correctors, etc).
- Initialize coarse level fields.
- Each coarse-scale integration point is mapped to the fine scale (via a local solution to a PDE).
- Once fine scale quantities are computed, appropriate averages are taken and transferred back to the coarse scale.
- Conservation of linear momentum is solved with those averages producing a new iterate for the coarse fields.

An example of the methodology is in Fig. 5.

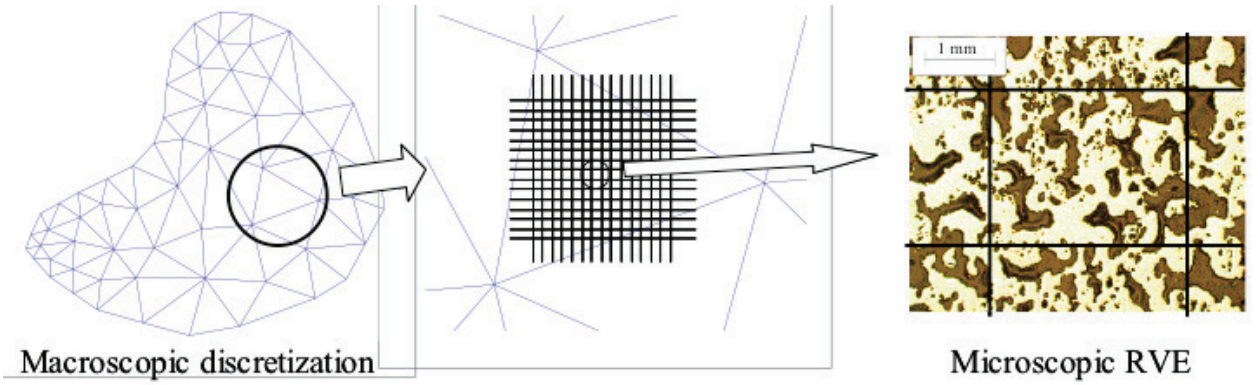

Fig. 5. Multiple scales

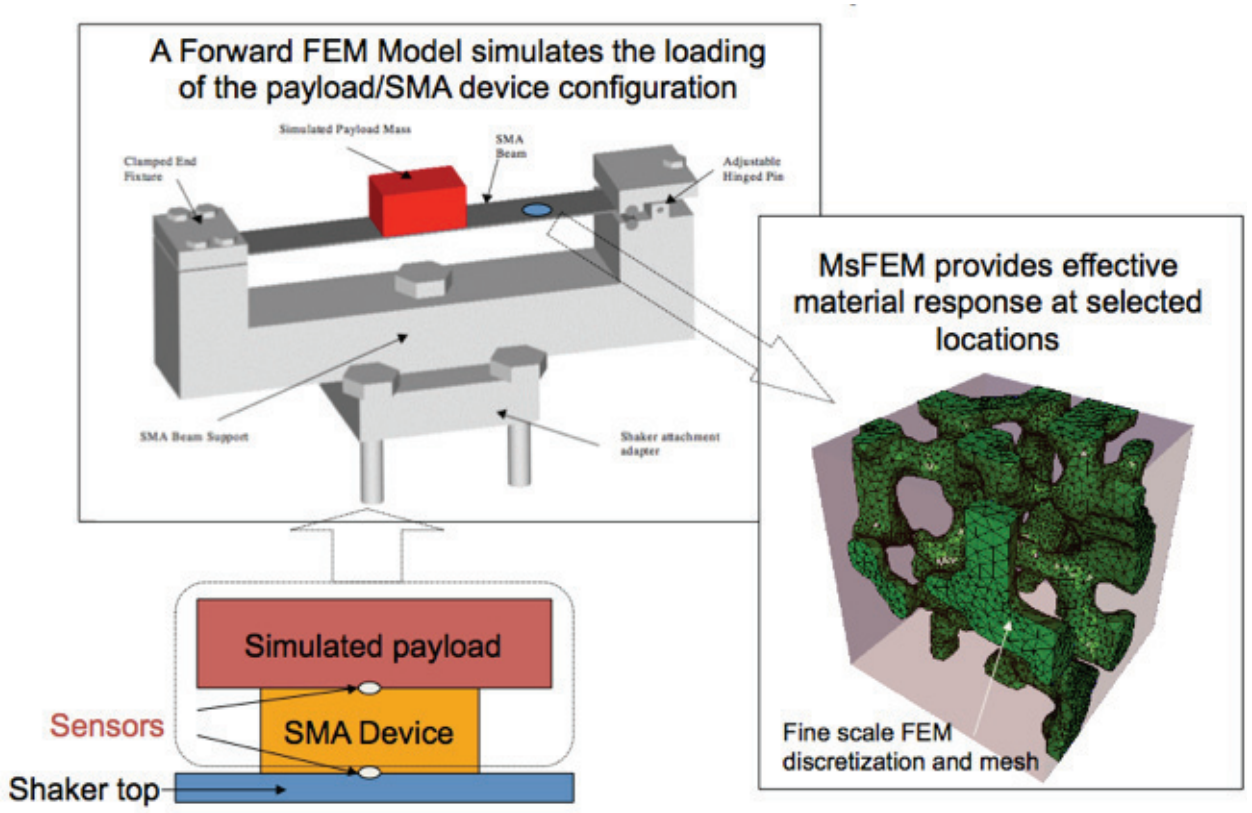

Fig. 6. Shaker and discretize SMA

4. Virtual Shaker and DDDAS Environment

Instead of designing a completely general virtual shaker device, we have concentrated initially on a specific device, namely a vibrating system consisting of a pseudoelastic SMA beam in a cantilevered-pinned configuration is being proposed. A mass is clamped at the center of the beam and the entire system is subjected to periodic vibrations over a range of frequencies in order to determine its isolation and damping capabilities (Fig. 6). This device is a simpler system compared to one with porous SMA components because the SMA constitutive model can be applied directly to modeling the response of the SMA. This allows elimination of the homogenization step of the porous material and thus reducing the uncertainties in the analysis and design of the system.

The use of a simple dense SMA beam in a dynamic system allows the investigation of the presence of phenomena that only occur in intrinsically nonlinear materials and cannot be observed in linear systems. Chaos (a long-term unpredictability in the response) is one of these phenomena. Nonlinearity, sensitive dependence on initial conditions, and at least three state variables are some intrinsic characteristics that a dynamical system must have present in order to induce chaos. Since chaotic behavior should be avoided in vibration isolation devices, this aspect requires thorough investigation.

The real shaker device we have access to produces data from its sensors every 0.1 seconds. If we change the sensors or their settings, we can get data at any rate available on market available sensors. The advantage of the virtual shaker is that we can adjust the data rate dynamically in order to determine how often we need data from a

real shaker device. Hence, the virtual environment can easily influence the lab environment or in a deployed product in an extremely cost effective manner.

The DDDAS components are preliminary at this stage of the project. It will be realized primarily by changing the temperature of the specimen dynamically to modify its general hysteresis properties, either the resistive heating and/or the fluid flow rate. We can also change the effective mechanical response by modifying the fluid pressure. We can respond to long-term fatigue changes in dense SMA model parameters. We can calibrate and improve microscale (dense) SMA model parameters based on dynamic data, e.g., the maximum transformation strain, transformation temperatures, etc. The DDDAS components interact with the forward simulations of the shaker/device setup to manage data streams and feedback control.

5. Conclusions and Future Work

In this paper we described our initial efforts to develop a DDDAS for porous SMAs and a virtual shaker device that will allow us to inexpensively design an experimental environment to validate our work. We have access to a real shaker device of the type simulated, but the virtual environment allows inexpensive tests to be run to determine how many sensors and the data rates that are needed for different porous SMAs and shaking situations without the expenses of people in the laboratory or the equipment therein. Additionally, we will develop a version of the DDDAS with stochastic variations in SMA response times and still need to validate the virtual DDDAS environment. Both will be reported on in the future.

Acknowledgements

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