Data Driven Design of Load Bearing Components

VI semester B.Tech Project Thesis report

Department of Mechanical Engineering

by

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Contents

Chapter 1

Data Driven Design: Introduction and motivation

In engineering, design refers to the method or process of solving problems. A proposed design offers solutions to an issue that leads to the creation of a product or process. Engineering design is the method of using our knowledge of mathematics and natural sciences to devise a device, part, or process to meet desired needs.

Mechanical design focuses primarily on the design of load bearing components with the aim of determining the best size, shape, and material to ensure the component's protection under load. As a result, a mechanical design procedure has often been carried out using relevant constitutive models in the past. These constitutive models have historically been important for structural design and material certification, and have been accomplished primarily through uni-axial tests aimed at determining elastic material properties.

1.1 Limitations of constitutive models

The aforementioned constitutive models which form the basis of mechanical properties

used for traditional design problems, have their own limitations. These models are complex and slow to process when dealing with complex problems for systems with high dimensional design variables. In certain cases, the design domain is much too large for a constitutive model to handle.

The nonexistence of knowledge of a design problem also makes getting to the correct constitutive model almost impossible. Constitutive models bring with them material modelling empiricism, modelling error and uncertainty. This modeling error and uncertainty arise from imperfect knowledge of the functional form of the material laws, the phase space in which they are defined, and from scatter and noise in the experimental data. Furthermore, often the models used to fit the data are ad hoc, without a clear basis in physics or a mathematical criterion for their selection, and thus the process of modeling is mired in empiricism and arbitrariness. The entire process of empirical material modeling, and model validation thereof, is open-ended and no rigorous mathematical theory exists to date that makes it precise and quantitative.

1.2 Data Driven Design

Previous work in using large unstructured data-sets to infer solutions for boundary value problems have been categorized under *Data Science*, but typically with the aim of parametric identification, or augmenting and automating, rather than replacing, the use and generation of material models. Material informatics uses database techniques to first identify parameters of correlation and then use machine-learning regression techniques to ultimately provide predictive quantitative models. Principal-component analysis provides methods of dimensional reduction that allow such modeling techniques to be applied.

In more recent research, Data-Driven Design is proposed as a way to remove the epistemic uncertainties associated with conventional constitutive models. Data driven design can minimise modelling error and uncertainty by avoiding empirical models, and there is no loss of experimental knowledge. A data-driven model-free approach can not only eradicate the explicit postulation of a particular constitutive model, but it can also produce databases of material states that follow some relevant sampling guidelines. Further, for orthosis and prostheses, the designs that are data –driven are more engaging and tailored to users' preferences. In data driven design where a large number of relevant data is collected and processed to be used as the model (guiding the behavior of the component instead of constitutive model) for design, instead of using data just a means for automating the analytical processes of already established design methodology using constitutive models.

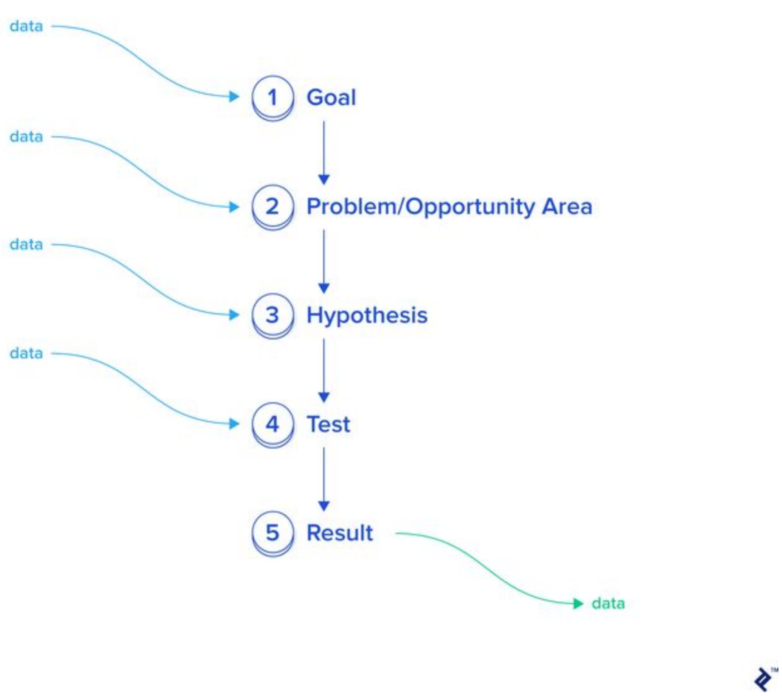

Fig. 1.1 Data Driven Design process flow

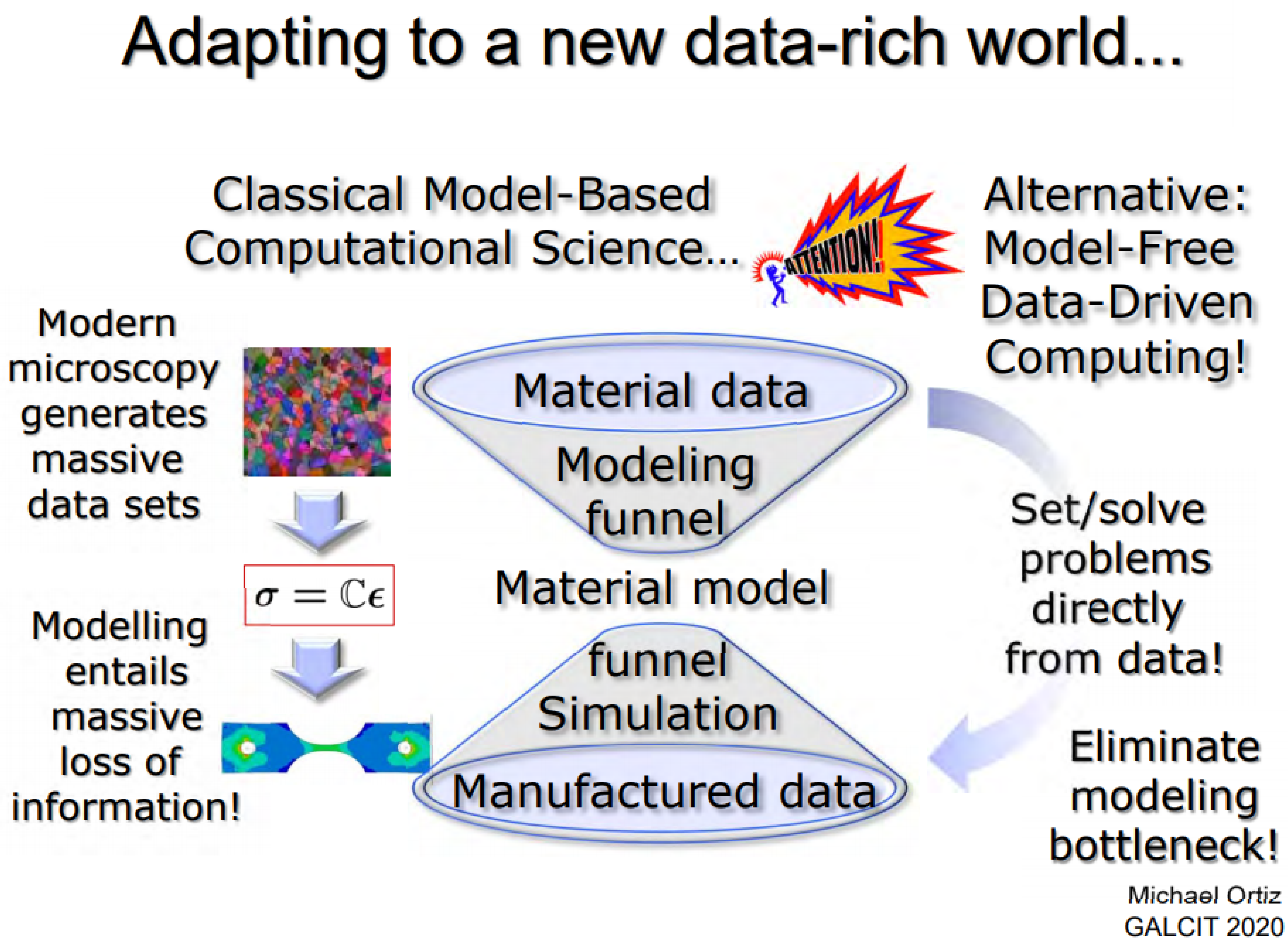

Fig. 1.2 Use of Model-Free design practices using material data

Chapter 2

Review

2.1 Literature review

Stainier et al [1] propose an integrated model-free data-driven approach to solid mechanics and show how principles and techniques of data driven computational mechanics leads to elimination of epistemic uncertainty linked to traditional constitutive models. Qualitative as well as quantitative results obtained using a data-driven approach were more accurate. The methodology proposed in the paper is to generate a material database using the Data-Driven Identification method, which is used to solve the classical boundary value problem. This is done by employing a distance minimization algorithm to find a compatible mechanical state (stress-strain field) in equilibrium, broadly termed as Data-Driven Computational Mechanics (DDCM). Acquired data is used to train a model to predict responses from different geometric structures of the same material. This method thus eliminates the postulation of a constitutive model entirely, thus getting rid of its uncertainties.

The paper follows this procedure and applies the DDI+DDCM methodology along with computational techniques such as FEM, to generate a robust procedure for response prediction. They work on two structural examples of the same material and document the performance of the constitutive models v.s the model-free technique, noting the errors as well as deviance and convergence of error distances with the difference in data points. The paper concludes to note that the performance of the data-driven technique is noteworthy for linear systems corresponding to standard elasticity problems, and would work just as fine for material non-linearity in the data-set, as our linear system of equations in the DDI+DDCM algorithms remain unaffected. We shall explore this paper further in detail throughout our report.

Shin et al. [2] presents a data-driven approach for developing a one-dimensional thin-walled beam model. In order to analyze complicated deformations occurring in a thin-walled beam by a beam theory, it is important to identify core cross-sectional deformations that are the bases for the one-dimensional beam analysis. For data processing, they have used principal component analysis to obtain the desired core cross-sectional deformations without making any assumptions about the behaviour of the beam's sectional deformations.

The core cross-sectional deformations can then be expressed in explicit functional forms (shape functions) to make the one-dimensional higher-order beam analysis construction easier. This paper discusses in detail the formulation of a robust Data-Driven pipeline to solve for design problems, and also the various levels and stages of processing raw material data for optimised use-cases. These practices were put to use by comparing numerical results with the processed shape functions obtained earlier, proving to show accurate results for static problems as well as vibration and buckling analyses. They have gone on to note the importance of correct procedure for the generation of data and further preprocessing. They have also stated that while their results have been obtained exclusively on tests for linear isotropic materials, they should be effective while dealing with composite materials as well.

Kirchdoerfer et al. [3] developed a new computing paradigm known as data-driven computing, in which calculations are performed directly from experimental material data as well as relevant constraints and conservation laws, such as compatibility and equilibrium, bypassing the empirical material modelling phase of traditional computing entirely. Data-driven solvers try to allocate the state from a predefined data set that comes closest to satisfying the conservation laws to each material point. These try to find the state that is nearest to the data set while satisfying the conservation laws. The resulting data-driven problem thus consists of the minimization of a distance function to the data set in phase space subject to constraints introduced by the conservation laws. They have checked the performance of this model-free approach by employing two examples- static equilibrium of 3D trusses and finite-element discretized linear-elastic solids. After the formulation of the constraint equations using Lagrange multipliers, they go on to capture the intersection of the constraint set with the global phase-space. With the use of Big Data, this paper discusses the scope of extending these design problems beyond linear isotropic materials, as well as exploring a data-driven approach for tackling dynamic problems since the addition of non-inertial forces will not affect the material behaviour.

2.2 Conclusion

The aforementioned papers shed more light into the conditions and criterion under which a model-free data driven design methodology would be more preferred over traditional modeling using the constitutive relations. In our report, we shall discuss one such methodology where we employ a similar distance-minimization algorithm to further predict the response of different geometric structures of the same material from a given phase space.

Chapter 3

Objective and work-plan

3.1 Methodology

The model-free approach we will look at, known as data-driven computational mechanics (DDCM) [3], involves formulating calculations directly from experimental material data and relevant critical constraints and conservation rules, bypassing the need for empirical material modelling in traditional computing. The data-driven solver aims to allocate the closest possible state from a predefined material-data set to and material point of the computational model while also meeting the necessary constraints and conservation rules. The local state assignment's best fit is calculated using a figure of merit that penalises the distance from the data set in phase space.

The resulting data-driven problem thus consists of the minimization of a distance function to the data set in phase space subject to constraints set forth by the essential constraints and conservation laws. We can also generate reference solutions using Finite-Element Analysis and constitutive models to benchmark the DDCM solver's performance.

DDCM has also been documented to be robust in its capacity to perform simulations on various geometries and loadings using a given database. Qualitatively, the method requires only limited data to predict the major features of strain and stress fields (e.g. location of maximal values). Quantitatively, the precision obtained depends directly on the quality of the database (number and sampling of data points).

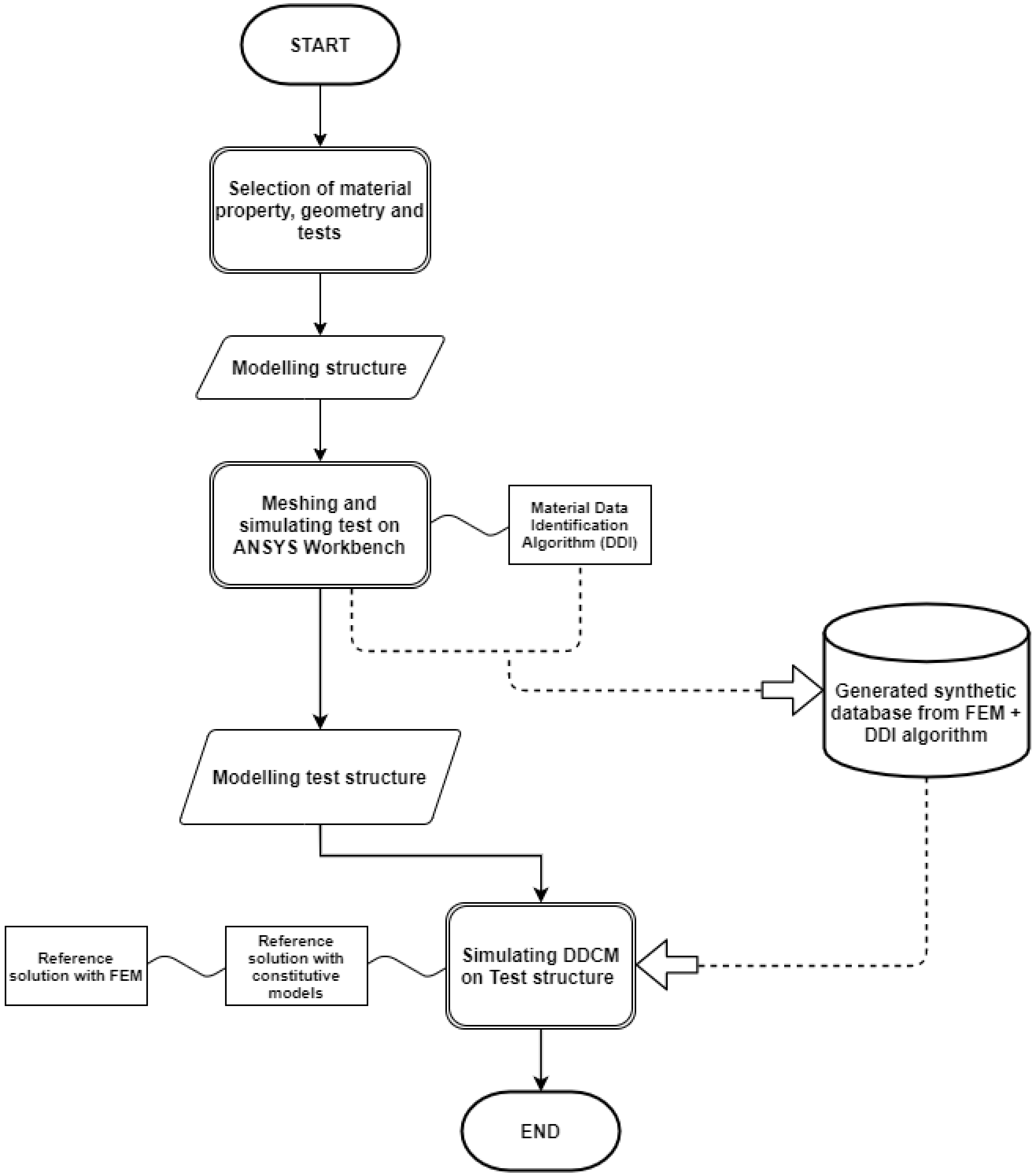

Fig. 3.1 Flowchart for the model-free method of solving a given mechanical design problem.

3.2 Distance-Minimization paradigm on material data-set

We consider discrete, or discretized, systems consisting of N nodes and M material points. Such systems typically arise from Finite Element (FE) discretization.

The system undergoes displacement $u = \{u_a\}_{a=1}^{N}$, with $\mathbf{u}_a \in R^{n_a}$ and n_a the dimension of the displacement at node a, under the action of applied forces $\mathbf{W} = \{\mathbf{f}_a\}_{a=1}^{N}$, with $\mathbf{f}_a \in R^{n_a}$. The local state of the system is characterized by stress and strain pairs $\{(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e)\}_{e=1}^{M}$, with $\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e \in R^{m_e}$ and m_e e the dimension of stress and strain at material point e. We regard $\mathbf{z}_e = (\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e)$ as a point in a local phase space $Z_e = R^{m_e} \times R^{m_e}$ and $\mathbf{z} = \{(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e)\}_{e=1}^{M}$ as a point in the global phase space $Z = Z_1 \times \cdots \times Z_M$.

The internal state of the system is subject to the compatibility and equilibrium constraints of the general form:

$$\boldsymbol{\varepsilon}_e = \mathbf{B}_e \mathbf{u}, \quad e = 1, \ldots, M \tag{3.1}$$

$$\sum_{e=1}^{M} w_e \mathbf{B}_e^T \boldsymbol{\sigma}_e = \mathbf{f} \tag{3.2}$$

where $\{w_e\}_{e=1}^{M}$ are elements of volume and $\mathbf{B}_e$ is a discrete strain operator for material point e.

This defines a subspace E constrained to the conditions (3.1) and (3.2), i.e

$$E = \{\mathbf{z} \in Z : (3.1)\ and\ (3.2) \tag{3.3}$$

The material behaviour we are dealing with is only known through a material dataset D_e of points $\mathbf{Z}_e = (\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e) \in Z_e$ obtained either experimentally or through some synthetic means, in the scope of our methodology.

A class of Data-Driven problems consists of finding the compatible and equilibrated internal state $\mathbf{z} \in E$ that minimizes the distance to the global material data set D = D1 ··· DM . To this end, we metrize the local phase spaces Z_e by means of norms of the form:

$$|\mathbf{z}_e|_e = \left(C_e \boldsymbol{\varepsilon}_e \cdot \boldsymbol{\varepsilon}_e + C_e^{-1} \boldsymbol{\sigma}_e \cdot \boldsymbol{\sigma}_e\right)^{1/2} \tag{3.4}$$

The local norms induce a metrization of the global phase Z by means of the global norm:

$$|\mathbf{z}| = \left(\sum_{e=1}^{M} w_e |\mathbf{z}_e|_e^2\right)^{1/2} \tag{3.5}$$

with associated distance:

$$d(\mathbf{z}, \mathbf{y}) = |\mathbf{z} - \mathbf{y}| \tag{3.6}$$

for y, z Z. The distance-minimizing Data-Driven problem is then,

$$\min_{\mathbf{y} \in D} \min_{\mathbf{z} \in E} d(\mathbf{z}, \mathbf{y}) = \min_{\mathbf{z} \in E} \min_{\mathbf{y} \in D} d(\mathbf{z}, \mathbf{y}), \tag{3.7}$$

i.e., we wish to find the point y D in the material data set that is closest to the constraint set E of compatible and equilibrated internal states or, equivalently, we wish to find the compatible and equilibrated internal state z E that is closest to the material data set D[3].

3.3 Data Driven solver

The aim of the Data Driven solver is to arrive at a compatible strain field and equilibrated stress field closest to the material data-set. Let us begin the DDCM analysis by taking a look at the formulation of these compatibility and equilibrium constraints.

The compatibility constraint can be enforced directly by introducing a displacement field u. The equilibrium constraint can then be enforced by means of Lagrange multipliers representing virtual displacements of the system.[2]

Compatibility Constraint: $\varepsilon_e = \mathbf{B}_e \mathbf{u}, \quad e = 1, \dots, M$

Equilibrium constraint: $\sum_{e=1}^{M} w_e \mathbf{B}_e^T \sigma_e = \mathbf{f}$

The Corresponding Euler-Lagrange equations are:

$$\begin{aligned} \left(\sum_{e=1}^{M} w_e \mathbf{B}_e^T C_e \mathbf{B}_e \right) \mathbf{u} &= \sum_{e=1}^{M} w_e \mathbf{B}_e^T C_e \varepsilon_e^* \\ \left(\sum_{e=1}^{M} w_e \mathbf{B}_e^T C_e \mathbf{B}_e \right) \boldsymbol{\lambda} &= \mathbf{f} - \sum_{e=1}^{M} w_e \mathbf{B}_e^T \boldsymbol{\sigma}_e^* \end{aligned} \tag{3.8}$$

which define two standard linear displacement problems. The closest point $\mathbf{z} = P_E \mathbf{y} \in E$ then follows as:

$\boldsymbol{\varepsilon}_\epsilon = \mathbf{B}_e \mathbf{u}, \quad e = 1, \dots, M$ $\qquad (4a)$

$\sigma_\varepsilon = a_e^* + C_r \mathbf{B}_e \lambda, \quad e = 1, \dots, M$ $\qquad (4b)$

A simple Data-Driven solver then consists of the fixed point iteration:

$$\mathrm{x}_{j+1} = P_E P_D \mathbf{z}_j \tag{3.9}$$

for $j = 0, 1, \dots$ and $z_0 \in Z$ arbitrary, where P_D denotes the closest point projection of a point in Z onto D. Ineration first finds the closest point $P_D \mathbf{z}_j$ to $\mathbf{z}_j$ on the material data set D and then projects the result back to the constraint set E. The iteration is repeated until $P_D \mathbf{z}_{j+1} = P_D \mathbf{z}_j$, i.e., until the data association to points in the material data set remains unchanged. Equation (3.8) define two standard linear elasticity problems, which can be interpreted as follows. The first states that displacement field should be compatible with material strains $\{\varepsilon_i^*\}$ in a weak sense, i.e. strains computed from $\mathbf{u}$ at material points associated to the same data point ε_i^* should average to that value. In view of the second part or $(4b)$, Lagrange multipliers λ can be interpreted as a discrete displacement field corresponding to the mismatch between mechanical and material stresses, resp. σ_e and σ_e^*. From a practical point of view, the above linear elasticity problems can be treated as classical problems, with arbitrary elastic properties $\mathcal{C}_e$ (possibly non-homogeneous), and subject to eigen-strain or eigen-stress fields. The system (3.8) corresponds to a linear elasticity problem with homogeneous kinematic boundary conditions, where the physical loading is applied (body forces and static boundary conditions) together with a field or eigen-stresses (or residual stresses) described by $\{\sigma_s^*\}$.

The Data-Driven paradigm has been extended to dynamics, finite kinematics and objective functions other than phase-space distance. These data-driven problems are well-posed and have properties of convergence with respect to the data-set.

Chapter 4

Data Driven Simulation

4.1 Data generation and Implementation

The material data-set is generated through simulations of load bearing members on computer software, namely ANSYS. For the purpose of this project, A finite element simulation was run on a thick plate(E=217.5E+09, Poisson's ratio= 0.3) with dimensions 200x128x50 mm with eccentric holes in it was bi-axially loaded in the vertical and horizontal plane. We have used this generated data-set, whereas you can model this yourself using the DDI algorithm. In an ideal case, we should use all of these synthetic databases to compare our solutions and infer the best results.

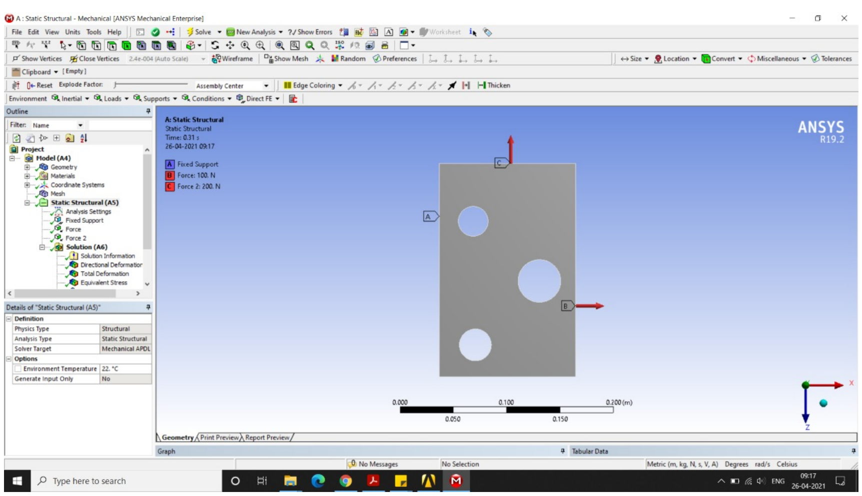

Fig. 4.1 Pre-meshed structure with loading conditions set up.

The plate was meshed with 300k+ nodes. From the loading displacement fields; stress and strain fields were generated over the entire volume of the plate. Next, we follow this up by the data-driven simualtion of a different mechanical problem of the same material, with the material data previously generated. Here, we will simulate a similar thick plate with a central hole. We modelled the mesh for this test structure similarly, this time with a relatively coarser mesh of 13K datapoints/nodes for computational convenience. The plate is subjected to a compression load in the vertical direction (average longitudinal strain of -0.4%). We should obtain a reference FEM solution at this step, with the help of the simulation software, which includes the total strain energy as well as our stress-strain space. These values will be useful to benchmark the performance of our model-free approach. With the help of the displaced mesh, we now run the DDCM algorithm on a local workmachine to fit this constrained space to the material data-set i.e the Phase space. Simulation was programmed in Python language code- thus helping us use it's mathematical library functions and packages. These include- Sci-Kit Learn for SGDRegressor, scaling and pipeline; SciPy and various plotting tools such as matplotlib and seaborn. Our hosted repository for this project can be viewed and contributed to at Github.

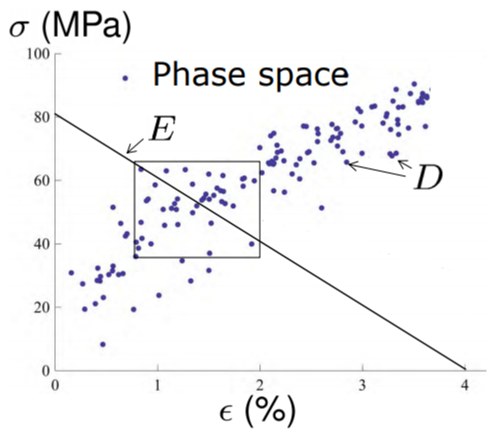

Fig. 4.2 Intersection of the constraint set over the phase-space

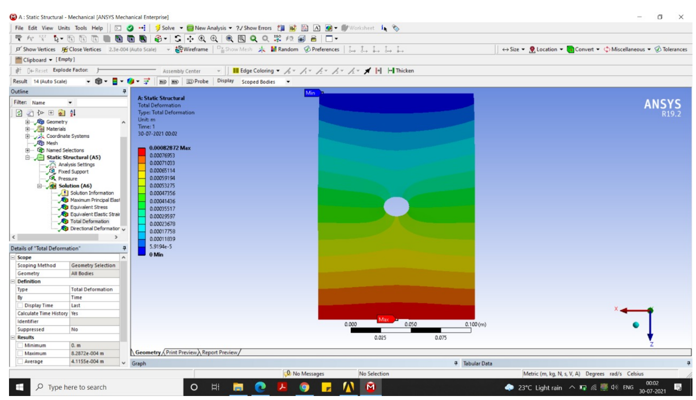

Fig. 4.3 Directional displacement of the test structure

4.2 Results

The sampled stress-strain space obtained was consistent with the isotropic hookean nature of our material piece used to generate the phase space (E = 217.5 GPa, ν = 0.3, plane strain). The exported results can be viewed in the following CSV file here.

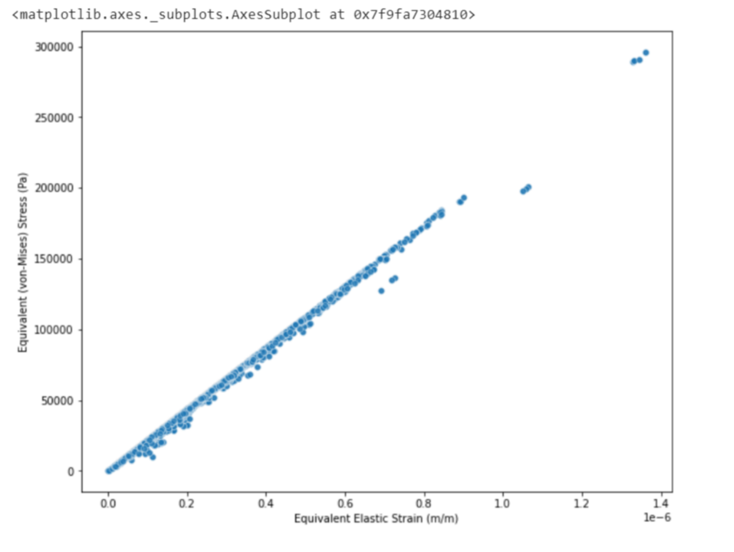

Fig. 4.4 Set of stress-strain states obtained

The total strain energies obtained through our different sources are a good indicative of the performance of each model. We wish to minimize the distances of energy (in J) between these results to check on the performance of DDCM and FEM results. We can also check the relative error between the DDCM and FEM results with respect to the local energy density over the constrained space.

We have found the mean of distances/error between the FEM and DDCM results corresponding to the stress field to be in the order of 10^2 J.

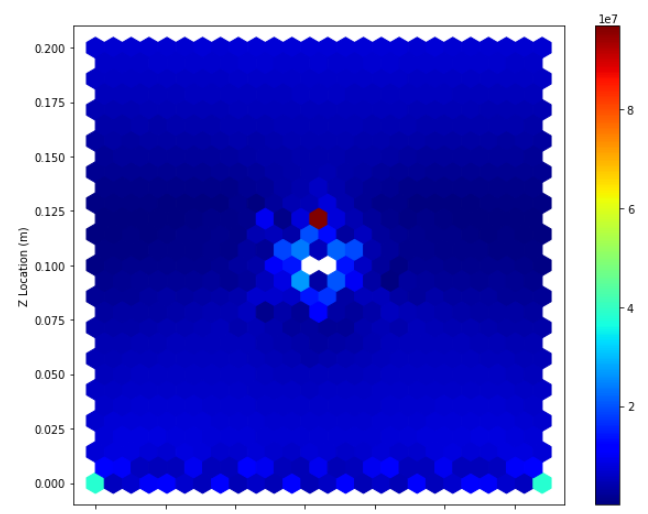

Fig. 4.5 Distance between FEM and DDCM solutions

Chapter 5

Future Work and References

5.1 Work for the upcoming semester

Over the course of two semesters we have extensively discussed various Data-Driven approach for solving mechanical design problems. We have also been able to generate synthetic data and simulate these results with selected model-free data driven techniques giving satisfactory performance. At this point, we want to tackle a particular design problem and assess all possibilities and solutions to accurately evaluate a data driven model. Our methodology will focus on understanding the universal and material laws associated with the design problem, generating/identifying a material data-set and finally applying the most relevant algorithms for the modelling step. Therefore in the upcoming semesters we shall focus on:

-Selection of a load bearing member and the material property behaviour we want to study. This should entail a design problem that is unfulfilled to certain extent with constitutive modelling. furthermore, we shall try to converge on a problem whose solution should prove to be beneficiary at any scope of engineering and health-care.

-Converge on a more inclusive methodology and pipeline for the selected design problem.

-Literature review of other Data Driven methodologies for solving design problems.

5.2 References

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