COMPUTATIONAL DESIGN OF DEFORMATION PROCESSES FOR THE CONTROL OF MICROSTRUCTURE-SENSITIVE PROPERTIES

A Dissertation

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by

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An important goal of modern manufacturing research and development is to determine the optimal means of producing reliable products. The design criteria vary depending upon the product requirements and the establishment of this criteria requires accurate description of various deformation mechanisms. The complexity of metal forming processes is apparent considering the coupled physical mechanisms like large deformation plasticity, processing induced microstructure evolution, thermal effects and damage. It is clear that several parameters and physical processes govern the product quality and it is impossible for a non-expert designer to consider all of them while making design decisions. In order to overcome this dependency on a small group of industry experts and to use the advances in computer and information technology, reliable optimization-based design techniques are developed as part of this thesis.

The physical and computational framework for the design methodology is developed in three stages. First, accurate modeling of physical phenomena occurring
during thermo-mechanical processing is developed. This includes the development of models for large deformation polycrystal plasticity, thermal effects and damage evolution during processing. Second, a novel, efficient and mathematically rigorous computational framework, called the continuum sensitivity method (CSM), is developed to evaluate the shape as well as non-shape (parameter) sensitivity of finite thermo-inelastic deformations. Finally, the developed techniques are combined to address realistic industrial design problems. Additionally, these techniques are extended towards design and control of multi-length scale problems, where design of microstructure sensitive properties (and texture in particular) is addressed. The highlight of this multi-length scale design framework is that the design variables are chosen to characterize macro-scale deformation. Accurate modeling and control of microstructure-sensitive material response is shown to be feasible through a set of exploratory examples. The thesis concludes with a discussion of possible developments and extensions to the proposed techniques.
Biographical Sketch

The author was born in Madras, India in August, 1979. After completing his high school education from Hindustan Aeronautics Limited (H. A. L.) Senior Secondary School in Hyderabad, the author was admitted into the Bachelor’s program at the Indian Institute of Technology, Madras in 1996, from where he received his Bachelors in Technology degree in June, 2000. In August 2000, the author was admitted into the doctoral program at the Sibley School of Mechanical and Aerospace Engineering, Cornell University and was awarded a special Masters degree in May 2003.
This thesis is dedicated to my parents Dr. M. G. Subramanian and Alamelu, and my brother Baskar for their constant support and encouragement towards academic pursuits during my school and college years.
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The metal forming design simulator developed as part of this thesis, was written using the object oriented programming environment of Diffpack and the academic
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Chapter 1

Introduction

Metal forming is a process in which an initially simple billet or sheet blank is physically deformed between dies to obtain a desired final configuration. Even though this operation sounds simple, the physical principles governing this phenomenon are quite complex; the metal flow, friction and contact at the tool-die interface, heat generation and transfer during plastic deformation and the relationship between microstructure, properties and processing are difficult to predict and analyze. In the late 1950s, a number of approximate methods of analysis were developed and applied to forming processes; these methods include the slab method, the slip-line field theory and Hill’s general method. These techniques were able to highlight essential aspects of the metal forming process, but were insufficient for practical design purposes. The early 1990s saw a sharp increase in the use of computer-aided engineering, manufacturing and design technologies and this trend seems to be towards an even wider application of technology for process simulation and design. More recently, the finite element method has been successfully applied to forming process modeling and detailed finite element simulations have gradually become the norm of the day. These simulations have come to play a vital role in materials processing and
account for coupled non-linear mechanisms like large deformation plasticity, varying contact and frictional conditions, and thermal effects and dissipation among others.

The significant objective behind analysis is to assist the metal forming engineer in the design of forming and preforming stages. Such design consists of (a) establishing kinematic relationships to predict metal flow; (b) establishing limits to ensure product with defects and damage within tolerable range; and (c) predicting the required loads and stresses, geometries of dies and workpieces to execute the forming process most effectively. Consequently, a systems approach was developed where the metal forming system consists of all input variables (geometry and material) related to the billet and dies, the conditions at the tool-billet interface, mechanics of plastic deformation and the characteristics of the finished product. Such an approach allows for the study of the effects of process variables on process economics and product quality. The key parameters affecting the success of metal forming operations include the control of metal flow and this is directly affected by material variables like the flow stress (with a given microstructure), workability etc. Infact, it is now well understood that the properties of a metal are strongly influenced by its microstructural features. Furthermore, during thermo-mechanical deformation processes, materials experience significant microstructural changes which in turn affect their mechanical properties and processing conditions.

In spite of this increased use of computer and information technologies in the analysis of thermo-mechanical processes, selection of actual process design variables still requires a significant amount of expert knowledge that is commonly obtained only through experience. To overcome this dependency on a small group of industry experts and to reach robust and less expensive designs, reliable optimization-based design techniques for thermo-mechanical processing are being developed. It has
been realized that the high cost of manufacturing critical structural components can be greatly reduced with the development of mathematically and physically sound computational methodologies for process design and control. Metal forming design, therefore, requires an accurate description of the thermo-mechanical deformation mechanisms in order to simultaneously achieve two or more of the design objectives defined in Box 1. Such design objectives are subject to processing constraints like maximum press capacity, zone of processing temperatures, final product quality and cost. These objectives can be achieved by proper design of the initial shape of the workpiece, the shape of the die, the ram speed, the initial state of the workpiece and die and other process parameters. Following [1], a process sequence design is assumed to involve the specific identification and selection of design variables in each of the underlying processing operations. Such intermediate processing stages help the designer by introducing more flexibility in the design process.

- Minimization of material usage
- Uniform deformation in the final product
- Minimum required work or forming force
- Desired microstructure in the final product
- Minimum or desired residual stress distribution
- Minimum deformation and wear of the die
- Desired shape of the final product
- Minimum porosity in the final product

Box 1: Objectives in hot forming design.

This thesis addresses the development of a mathematically and computationally rigorous gradient-based optimization methodology for a virtual materials process design simulator that is based on quantified product quality and accounts for process
targets and constraints. This virtual design simulator, depicted in Box 2, includes the development of a continuum sensitivity analysis consistent with the virtual direct process simulator and is capable of accurately computing the gradients of objective functions and process constraints.

- 1. Mathematical representation of the design objective
- 2. Selection of the sequence of processes (stages) and initial process parameter designs using knowledge based expert systems, and/or microstructure classification techniques.
- 3. Selection of the design variables (e.g. parametric representation of dies/preforms)
- 4. Selection of a virtual direct process model
- 5. Interactive optimization environment
- 6. Continuum multi-stage process sensitivity analysis consistent with the direct process model

Box 2: A computational design simulator for forming processes.

In developing a design simulator, questions regarding the robustness and reliability of the design process and final product can also be addressed through a realistic process simulator. This needs incorporating damage effects, as most macroscopic failures in metals occur due to damage accumulation during thermo-mechanical processing. Hence, it is necessary to predict ductile fracture and design processes which avoid or limit damage in the finished product. It is also well understood that the properties of a metal are strongly influenced by its microstructural features like the grain size, the crystal orientation and texture. During thermo-mechanical deformation processes, materials experience significant microstructural changes which in turn strongly affect their mechanical properties. The main reason for this re-
newed interest in process design technology, lies in the attractiveness of control of microstructural properties in metallic materials by processing rather than by alloying - the current, expensive industrial practice. There have been extensive efforts, over the years, to understand the physics behind the evolution of microstructure. The stored energy was established as one of the important driving forces behind recrystallization. In a crystalline solid, the free energy of the material is increased during deformation by the presence of dislocations. On annealing however, the microstructure and the properties may be partially restored by the process of recovery. Recrystallization is a further restoration process wherein new, dislocation free, grains are formed within the deformed microstructure. Recrystallization may also take place during deformation at elevated temperatures and is termed as dynamic recrystallization. The emphasis in this work is on modeling and control of dynamic recrystallization occurring in metals during hot forming operations. The main parameters which have been identified to affect recrystallization include kinetics, straining rates and temperature. The key literature, which describes recrystallization, affecting parameters and methods of control include [2, 3]. The developed analysis, for dynamic recrystallization, follows an earlier effort by Busso [4] where a continuum theory for dynamic recrystallization was developed based on a hypoe-elastic framework.

Extending the design and control process to polycrystalline materials is critical as most industrial applications involve materials that are polycrystalline in nature. The properties of polycrystalline materials depend not only on the properties of the individual crystals but also on parameters like the crystallographic orientation (texture) that characterize the polycrystal. This texture characterizes the mechanical, optical and magnetic behavior of the material. For example, earring during
deep drawing of cups/cans along with variations in thickness of the cups/cans is attributed to anisotropy [5]. Texture and anisotropy have their advantages too, as appropriate textures block the propagation of cracks or make a material magnetically/optically superior in particular directions. The vastness of fields wherein texture affects properties makes it an interesting, challenging and industrially important problem [6, 7].

Polycrystal models have primarily characterized the polycrystal through a discrete aggregate of crystals, see for example [8]-[15]. These approaches work on the idea of combining discrete, preselected, single crystal responses with a suitable macro-micro linking hypothesis. Such discrete aggregate models, though simple, do not characterize texture effectively. There also exists no means by which one can compare and quantify differences between textures associated with distinct discrete aggregates. An alternate approach is a continuum representation, wherein texture is described through an orientation distribution function (ODF) which expresses the density of crystal orientations over the space of orientation parameters [16]. Common methods of ODF representation include series expansion using generalized spherical harmonics, infinite polynomial series or tensorial Fourier series [17, 18].

In [18], the authors discuss the design of a compliant beam so as to maximize the deflection without plastically deforming the beam. Analysis was performed using spectral methods which are complex and have global support thus providing no local control of the quality of the ODF. This tends to create problems in the context of sharp textures and requires significant number of terms in the series to obtain an accurate texture representation. Alternately Kumar and Dawson, in [19, 20], proposed the idea of representing the ODF with finite element polynomial functions defined over an explicit discretization of the orientation space (angle-axis parametrization)
which helped mitigate the numerous disadvantages of continuum representations.

In addition to the quantification of anisotropy, researchers have been interested to study the mechanisms for the evolution of plastic anisotropy and to formulate models that predict the experimentally observed behavior [17],[20]-[33]. Even though there is a wealth of knowledge available in this field, most polycrystal models are restrictive in the sense of a limited operating region of processing conditions. In practice, however, applications of interest lie in a very broad operating regime - from quasi-static strain rate applications to ballistic applications [10, 34]; and from cold rolling of plates to hot forging of engine components. Elastic effects have also been neglected in many studies [10, 15, 25] even though it has been shown [14] that elastic effects do play a significant role. More recently, Anand et al. in [8, 12] have developed improved kinetic equations for the shearing rates on slip systems and have compared the response for b.c.c Tantalum and f.c.c Aluminium with experimentally available results. This theory has been motivated based on the thermal activation theory for plastic flow and has been extended towards design in this thesis. As part of this thesis, fully implicit macro-micro (multi-length scale based) finite element models of deformation of polycrystal materials are introduced and implemented. This involved combining salient features from different methodologies to develop an advanced and accurate process simulator, discussed extensively in Chapters 2 and 4.

In the second part of the thesis, a framework for preform as well as process parameter optimization is proposed for multi-stage metal forming processes. The design of each individual process will be performed using gradient-optimization techniques that are based on a rigorous continuum sensitivity method (CSM). The continuum sensitivity method developed by Zabaras and colleagues, for single-stage
deformation processes [35]-[41] to compute the sensitivities of isothermal processes, has been extended to accommodate diverse physical phenomena occurring during thermo-mechanical processing. This development is discussed in detail in Chapter 3. One of the features of the sensitivity problem is its design-differentiate and then discretize approach, rather than the standard, discretize and then design-differentiate approach. In Chapter 5, multi-length scale sensitivity is defined and algorithms are proposed that allow for computing the sensitivity fields of microscopic quantities with respect to macroscopic design parameters. The computed sensitivities are validated and used in a gradient based optimization framework for the control of microstructure during deformation processes. The advantages of such an approach are substantial and are discussed as needed. The thesis concludes with brief directions and suggestions for future research efforts in modeling and design of thermo-mechanical processing operations.
Chapter 2

Phenomenological approach towards modeling deformation processes

The complexity of metal forming design is apparent considering the coupled non-linear physical mechanisms that need to be accounted for. These physical mechanisms include (a) large deformation plasticity, (b) deformation induced microstructure evolution, (c) time varying contact and friction conditions, (d) thermal effects and mechanical dissipation and (e) damage accumulation leading to material rupture. The role of these mechanisms in the processing of the initial workpiece, to yield the final product, is paramount and in almost all cases of design, intermediate processing stages need to be used to efficiently transform the initial geometry/material into the desired final shape (with specific properties). The present analysis of thermo-mechanical processes is based on a Lagrangian framework and includes both total Lagrangian (TL) and updated Lagrangian (UL) formulations. The research effort also includes full Newton-Raphson linearizations of the prin-
ciple of virtual work [42] and implementations of tangent stiffness matrices. The reader is referred to [43] for an insight into the state-of-art in finite deformation computational plasticity.

The general deformation problem with material and geometric nonlinearities is divided into a number of sub-problems like the kinematic, constitutive, contact and thermal sub-problems. The thermal and deformation problems are weakly coupled. The thermal field affects deformation through the effect of thermal expansion and dependence of mechanical response on temperature; the deformation field in turn affects the thermal field through dissipative plastic heating along with changes to the geometry of workpiece, porosity and the nature of the thermal boundary conditions. The direct problem can therefore be stated as follows: Compute the time history of the deformation, temperature and material state of a body deforming as a result of external forces and/or deformation due to contact and friction at the workpiece-die interface. Each of the sub-problems, namely the kinematic, constitutive and thermal sub-problems, are discussed in the following sections. The contact problem has been extensively described in [37].

2.1 Kinematic and constitutive framework

Consider \( B_0 \) as the initial configuration of the body (at time \( t = 0 \)) and \( B_{n+1} \) as the current configuration (time \( t = t_{n+1} \)). The reference configuration in an updated Lagrangian formulation is taken as \( B_n \) at time \( t = t_n \). Let \( X \) be a material particle in \( B_0 \) and \( x = \hat{\mathbf{x}}(X, t) \equiv \hat{\mathbf{x}}(\mathbf{x}_n, t) \) be its location at time \( t \in [t_n, t_{n+1}] \). The total deformation gradient, \( F_{n+1} \), is then defined in terms of the relative deformation
Figure 2.1: A kinematic framework for the constitutive modeling of thermo-inelastic deformations for porous media.

Gradient, $F_r$, as follows:

$$F_{n+1} = \nabla_0 \tilde{x}(X, t_{n+1}) = \nabla_n \tilde{x}(x_n, t_{n+1}) \nabla_0 \tilde{x}(X, t_n) = F_r F_n$$

(2.1)

In all following equations, the subscript $n+1$ will be omitted for fields defined on the current configuration and the subscript $n$ will be used to indicate the reference configuration $B_n$. In an appropriate kinematic framework for large deformation inelastic analysis, such as the one introduced in [44], the total deformation gradient is decomposed into thermal, plastic and elastic parts as:

$$F = F^e F^p F^\theta, \quad \det F^p > 0, \ \det F^e > 0, \ \det F^\theta > 0$$

(2.2)

where $F^e$ is the elastic deformation gradient, $F^p$ is the plastic deformation gradient and $F^\theta$ is the thermal part of the deformation gradient. A graphical representation of this constitutive framework is given in Figure 2.1. With the above constitutive framework, notions of an intermediate thermally expanded hot unstressed configuration and of an intermediate hot plastically deformed relaxed configuration are
introduced. Assuming isotropic thermal expansion, the evolution of the intermediate thermally expanded unstressed configuration is given by:

\[ \dot{F}^\theta F^{\theta -1} = \beta \dot{\theta} I \]  

(2.3)

where \( \beta \) is the thermal expansion coefficient and \( I \) is the second-order identity tensor. \( \det F^p \) is taken as a measure of internal damage. Applying balance of mass for the matrix material, one obtains the following:

\[ \det F^p = \frac{1 - f_o}{1 - f} \]  

(2.4)

where \( f_o \) and \( f \) represent the void volume fractions in the initial and deformed configurations, respectively. The hyperelastic constitutive equations are written as:

\[ \bar{T} = \mathcal{L}^e [\bar{E}^e] \]  

(2.5)

where the strain measure, \( \bar{E}^e \), is defined with respect to the intermediate (un-stressed) configuration as \( \bar{E}^e = \ln U^e \). The corresponding conjugate stress measure \( \bar{T} \) is the pullback of the Kirchhoff stress with respect to \( R^e \),

\[ \bar{T} = \det(U^e) R^{eT} T R^e \]  

(2.6)

Here \( U^e \) and \( R^e \) are calculated from the polar decomposition, \( F^e = R^e U^e \), of \( F^e \). For an isotropic material, the elastic moduli \( \mathcal{L}^e \) is given by:

\[ \mathcal{L}^e = 2\mu \mathcal{I} + \left\{ \kappa - \frac{2}{3}\mu \right\} I \otimes I \]  

(2.7)

where the shear modulus \( \mu \) and bulk modulus \( \kappa \) are, in general, functions of \( f \) and \( \theta \) [78, 79] and \( \mathcal{I} \) denotes the fourth order identity tensor. The equilibrium equation can be expressed on the reference configuration \( B \) as [45],

\[ \nabla_n \cdot P + f = 0 \]  

(2.8)
where $\nabla_n \cdot$ represents the divergence and $f$ is the body force expressed on the reference configuration. The Piola-Kirchhoff I (PK-I) stress is expressed as

$$ P = \det F_r T F_r^{-T} \quad (2.9) $$

and the deformation problem is solved incrementally in time starting from the given initial configuration $B_0$. In order to solve the equilibrium equations at time $t = t_{n+1}$, the constitutive relationship between the Cauchy stress $T$ and the relative deformation gradient $F_r$ and temperature $\theta$ should be evaluated. It is well known that the equivalent tensile stress $\sigma_m$ of the matrix material should be defined implicitly in terms of the Cauchy stress $T$ and the void fraction $f$ [46, 47]. With the assumption of isotropy, a particular form of this dependence is:

$$ \Phi = \Phi(\sigma_m, f, p, S) = 0 \quad (2.10) $$

where the dependence of the potential $\Phi$ on the stress $T$ is restricted to its first and second invariants. Here, $S$, the norm of the stress deviator, $\bar{T}' = \bar{T} + p I$, is given by

$$ S = \sqrt{\bar{T}', \bar{T}'} \quad (2.11) $$

where $p$ is the mean normal pressure given as

$$ p = -\frac{1}{3} \text{tr} \bar{T} . \quad (2.12) $$

The particular consistency condition used in this work is [47]:

$$ \Phi = \frac{3}{2} S^2 - 1 + 2q_1 f^* \cosh\left( \frac{3}{2} q_2 \frac{p}{\sigma_m} \right) - (q_1 f^*)^2 = 0 \quad (2.13) $$

with $q_1 = 1.5$ and $q_2 = 1.0$. The function $f^*(f)$, proposed to handle the loss in the load carrying capacity for void fractions greater than a critical value $f_c$, is taken
as:

\[
 f^* = \begin{cases} 
 f & \text{if } f \leq f_c \\
 f_c + (f_u^* - f_c)(f - f_c)/(f_f - f_c) & \text{otherwise} 
\end{cases}
\] (2.14)

where \( f_u^* = 1/q_1 \), \( f_f = 0.25 \) and \( f_c = 0.15 \) as proposed in [47]. In the limit of a fully dense solid, the function \( \Phi \) is such that, the classical \( J_2 \) von Mises isotropic plasticity theory is recovered, i.e., the following condition holds:

\[
 \lim_{f \to 0} \Phi = \left( \frac{(3/2)S^2}{\sigma_m^2} - 1 \right) \equiv 0
\] (2.15)

The void fraction, \( f \), and temperature, \( \theta \), are responsible for the loss in the load carrying capacity of the material. It is stressed that in the framework of the Gurson-Tvergaard-Needleman model, \( \dot{f} \geq 0 \) is not a restriction and void healing can be modeled.

Conservation of mass leads to the evolution equation for the void fraction and it has the form (see Equation (2.4)):

\[
 \dot{f} = (1 - f)tr(\bar{D}^p)
\] (2.16)

The evolution of the plastic part of the deformation gradient \( F^p \) is given by the normality rule,

\[
 \bar{D}^p = \text{sym} \left( \bar{L}^p \right) = \dot{\gamma} \partial_T \Phi = \dot{\gamma} \left[ (\partial_S \Phi) N - \frac{1}{3}(\partial_p \Phi) I \right]
\] (2.17)

where \( \bar{L}^p = \dot{F}^p F^{p-1} \) and \( N = \frac{T'}{S'} \) is the direction of the stress deviator. The spin in the intermediate, hot, unstressed, plastically deformed configuration is assumed to vanish (for isotropic materials) resulting in the following equations:

\[
 \bar{D}^p = \bar{L}^p \quad \bar{W}^p = 0
\] (2.18)

The work equivalence relation, \( T \cdot D^p = (1 - f)\sigma_m \dot{\varepsilon}^p \), is used to evaluate the plastic shearing rate \( \dot{\gamma} \) in Equation (2.17) as:

\[
 \dot{\gamma} = \frac{(1 - f)\sigma_m}{S\partial_S \Phi + p\partial_p \Phi} \dot{\varepsilon}^p
\] (2.19)
The evolution of the equivalent tensile plastic strain is specified via uniaxial experiments as

$$\dot{\varepsilon}^p = f(\sigma_m, s, \theta)$$ (2.20)

and the evolution of the isotropic scalar resistance \(s\) is also obtained from experiments and has the form,

$$\dot{s} = g(\sigma_m, f, p, S, \theta) = h(\sigma_m, f, p, S, \theta) \dot{\varepsilon}^p - \dot{r}(\sigma_m, s, \theta)$$ (2.21)

where \(\dot{r}(\sigma_m, s, \theta)\) is the recovery function. In the following analysis, the body is assumed to behave as a continuum despite the presence of microvoids. In addition, void nucleation is neglected and void growth is assumed to be the major damage mechanism. Finally, the material is assumed to have an initial finite porosity to trigger further development of defects.

### 2.1.1 Microstructure related length scales in phenomenological approach

Explicit microstructure related length scales can be introduced into the constitutive framework to model the dependence of the material behavior on its recrystallized state. The microstructure is described through internal state variables linked to the grain size as developed in [4, 48] (through a hypoelastic formulation). This extended constitutive framework is described in detail in [50]. For completeness, the ideas behind this approach is briefly summarized.

Dynamic recrystallization, i.e., recrystallization and recovery during deformation processing, is modeled through the approach discussed in [50]. The microstructure is described through internal state variables such as the mean grain size, \(L\) and volume fraction recrystallized, \(\chi\). Dynamic recrystallization is modeled in two
stages: primary and secondary recrystallization. Primary recrystallization is defined as the region of recrystallization that mostly involves grain refinement and secondary recrystallization as that region which involves grain growth. The evolution of the isotropic scalar resistance $s$, in this case, involves a dynamic recovery function, $\dot{r}(\sigma_m, s, \theta, L)$, associated with recrystallization, which describes the annihilation rate of dislocations. In addition, the evolution of the average grain size during and immediately after primary recrystallization (primary stage in dynamic recrystallization) is considered to be governed by (refer [50]):

$$\dot{L} = l(\sigma_m, s, \theta, L) = \dot{L}_{ref} + \dot{L}_{grow}$$

(2.22)

where $\dot{L}_{ref}$ is a function that describes the overall grain refinement taking place during primary recrystallization and $\dot{L}_{grow}$ represents the kinetics of grain growth process driven by grain boundary energies during secondary recrystallization.

### 2.2 Time integration of the constitutive problem

In the incremental constitutive problem, one evaluates the set $(T, s, f, F^p)$, with the body configurations at time $t_n, t_{n+1}$ and the set $(T_n, s_n, f_n, F^p_n, \theta)$ known. The reader is reminded that the subscript $(n+1)$ will be omitted for fields on the current configuration. Integration of the evolution equation for the plastic deformation gradient yields

$$F^p = \exp(\Delta t \dot{D}^p) F^p_n$$

(2.23)

where $\Delta t = t_{n+1} - t_n$. Integrating Equation (2.3) results in

$$F^\theta = \exp(\Delta t \dot{\theta} I) F^\theta_n$$

(2.24)

Based on Figure 2.2, the following can be observed:
Figure 2.2: Evolution of the various material configurations within a single time step as needed in the integration of the constitutive model.

\[
F_T = F^0 F^{0 -1}_n = \exp \left( \Delta t \beta \dot{\theta} I \right) \tag{2.25}
\]

\[
F_C = F^p F^p_n = \exp \left[ \Delta t \beta \dot{\theta} I + \Delta t \bar{D}^p \right] \tag{2.26}
\]

A trial elastic deformation gradient, \( F^e_* \), defined as \( F^e_* = F , F^e_n = R^e_* U^e_* \), is introduced. Further, from Figure 2.2, the following holds good:

\[
F^e_* = F^e F_C \tag{2.27}
\]

Polar decomposition of the above equation, while observing that \( F_C \) is symmetric, results in the following:

\[
R^e_* = R^e
\]

\[
U^e_* = U^e F_C \tag{2.28}
\]
Taking logarithms of this equation and using Equation (2.26), the following is derived

$$\bar{E}^e = \bar{E}_e^e - \Delta t \left[ \beta \dot{\theta} I + \bar{D}^p \right] \quad (2.29)$$

where the trial elastic strain is given as $\bar{E}_e^e = \ln U_e^e$.

From the hyperelastic constitutive equation (Equation (2.5)) and the flow rule (Equation (2.17)), the following equations for the deviatoric and pressure parts of $\bar{T}$ are derived as:

$$\bar{T}' = \bar{T}_s' - [2\mu \Delta t \dot{\gamma} \partial S \Phi] T_s' \quad (2.30)$$

$$p = p_s - \Delta t \kappa \dot{\gamma} \partial p \Phi + 3\kappa \beta \Delta \theta \quad (2.31)$$

where $\bar{T}_s'$, $p_s$ are the deviatoric and pressure parts of $\bar{T}_s = \mathcal{L}^e [\bar{E}_s^e]$, respectively, and $\Delta \theta = \theta - \theta_n$. From Equation (2.30) and the definition of $N$, the following statement can be made about the directions of the deviatoric stresses

$$N = N_s = \frac{T_s'}{S_s} \quad (2.32)$$

where $S_s$ is the norm of the trial deviatoric stress. As a result, the tensorial Equation (2.30) degenerates to a scalar equation involving the norms of the respective stress quantities with

$$\bar{T}' = \eta \bar{T}_s' \quad (2.33)$$

where $\eta$ is the radial return factor given by

$$\eta = \frac{S}{S_s} \quad (2.34)$$

The following scalar equations are then obtained:

$$S = S_s - 2\Delta t \mu \dot{\gamma} \partial S \Phi \quad (2.35)$$

$$p = p_s - \Delta t \kappa \dot{\gamma} \partial p \Phi + 3\kappa \beta \Delta \theta \quad (2.36)$$
Euler backward time integration of Equations (2.16) and (2.21) leads to the following:

\[ s = s_n + \Delta t \, g(\sigma_m, \mathcal{S}, s, \theta, f) \]  \hspace{1cm} (2.37)

\[ f = f_n - (1 - f) \Delta t \, \dot{\gamma} \partial_p \Phi \]  \hspace{1cm} (2.38)

Thus only the scalars, \( \sigma_m, \mathcal{S}, s, p \) and \( f \) need be evaluated. In addition to Equations (2.35)-(2.38), the set \( \{ \sigma_m, \mathcal{S}, s, p, f \} \) must satisfy the potential \( \Phi \) (Equation (2.10)). This system of equations is solved simultaneously, within a time step, using a Newton-Raphson procedure incorporating a line search algorithm. This was found to be very efficient for material models considered in the examples to be discussed later. With these values of parameters, the Cauchy stress is updated as:

\[ T = \exp \left( \frac{p_s}{\kappa} \right) R_s^e T R_s^{e T} \]  \hspace{1cm} (2.39)

with \( T = \eta \, T^r - p I \), where \( \eta \) is the radial return factor defined earlier. The time integration of the model incorporating grain size effects is described in [50], and follows along lines similar as those enumerated above.

### 2.3 The principle of virtual work

The solution of the deformation problem proceeds incrementally in time starting from the initial configuration \( \mathcal{B}_0 \). The solution of a generic loading increment involves the solution to the principle of virtual work (PVW) given as

\[ \int_{\mathcal{B}_n} P(\mathbf{F}_r) \cdot \nabla_n \hat{\mathbf{u}} \, dV_n = \int_{\Gamma_n} \lambda \cdot \hat{\mathbf{u}} \, dA_n + \int_{\mathcal{B}_n} f \cdot \hat{\mathbf{u}} \, dV_n \]  \hspace{1cm} (2.40)

for every admissible test function \( \hat{\mathbf{u}} \) expressed over the reference configuration \( \mathcal{B}_n \).

The vector \( \lambda \) is the current contact traction expressed per unit area in \( \Gamma_n \subset \partial \mathcal{B}_n \).
This weak form can be re-written as

\[ G(u_{n+1}, \tilde{u}) = G^{\text{int}}(u_{n+1}, \tilde{u}) - G^{\text{ext}}(u_{n+1}, \tilde{u}) = 0 \]  (2.41)

for every kinematically admissible test field \( \tilde{u} \) expressed over the reference configuration \( B_n \), where

\[ G^{\text{int}}(u_{n+1}, \tilde{u}) = \int_{B_n} P_r \cdot \nabla_n \tilde{u} \, dV_n \]  (2.42)

and

\[ G^{\text{ext}}(u_{n+1}, \tilde{u}) = \int_{\Gamma_n} \lambda_n \cdot \tilde{u} \, dA_n + \int_{B_n} f \cdot \tilde{u} \, dV_n \]  (2.43)

The incremental quasi-static boundary value problem at time \( t = t_{n+1} \) is to find the incremental displacement field \( u_{n+1} \equiv u(x_n, t_{n+1}) = \hat{x}(x_n, t_{n+1}) - x_n \) that will satisfy Equation (2.40). To solve the non-linear system for \( u(x_n, t_{n+1}) \), a Newton-Raphson iterative scheme along with a line search procedure is employed. Let \( u^{(j+1)}_{n+1} \) and \( u^{(j)}_{n+1} \) be the displacement fields at the end of the \( (j+1) \)th step and the \( j \)th step in the Newton-Raphson procedure. The linearized form of Equation (2.41) is

\[ G\left(u^{(j)}_{n+1}, \tilde{u}\right) + \frac{\partial G}{\partial u^{(j)}_{n+1}} \delta u^{(j)} = 0 \]  (2.44)

where \( \delta u^{(j)} = u^{(j+1)}_{n+1} - u^{(j)}_{n+1} \) is the full Newton step. The linearization of the term \( G^{\text{int}} \) is given as

\[ \delta G^{\text{int}} = \int_{B_n} \delta P \cdot \nabla_n \tilde{u} \, dV_n \]  (2.45)

where

\[ \delta P = \delta \left( \det F_r \, T \, F_r^{-T} \right) \]  (2.46)

Complete linearization of this term leads to the following [49]-[51]

\[
\delta P_r = \det F_r \left\{ \text{tr} \left( \delta F_r \, F_r^{-1} \right) \right\} T_{n+1} - T_{n+1} \left( \delta F_r \, F_r^{-1} \right)^T \\
- \text{tr} \left( \frac{1}{3\kappa} \, C \left[ \delta \bar{E}_s^e \right] \right) T_{n+1} + \exp \left( \frac{p_*}{K} \right) R^e \, C \left[ \delta \bar{E}_s^e \right] \left( R^e \right)^T
\]
\[ + \left( \delta \mathbf{R}^e (\mathbf{R}^e)^T \right) T_{n+1} - T_{n+1} \left( \delta \mathbf{R}^e (\mathbf{R}^e)^T \right)^T \right\} F^{-T} \]  

where \( C \) denotes the consistent tangent linearized moduli. These moduli are computed corresponding to the particular constitutive model and integration scheme used to represent the material behavior. The relationship between \( \delta \mathbf{F}_r \) and the primary unknown \( \delta \mathbf{u} \) is given as

\[
\delta \mathbf{F}_r = \delta \nabla_n \mathbf{x} = \nabla_n (\delta \mathbf{x}) = \nabla_n (\delta \mathbf{u})
\] (2.48)

The above weak form is solved in an incremental-iterative manner as a result of material as well as geometric non-linearities. The finite element method is used for the solution of the weak form and in the present work, bilinear quadrilateral elements are used along with the assumed strain analysis described in [41]. The augmented Lagrangian formulation of Laursen and Simo [43] is used to model contact and friction. The implementation of contact algorithm is discussed in detail in [40]. The solution process for the system described by Equation (2.44) is described in detail in [51].

### 2.4 Thermal sub-problem

In the absence of external heat sources, the balance of energy in the current configuration \( B_{n+1} \) of the workpiece takes the following form:

\[
\rho c \frac{\partial \theta}{\partial t} = \mathcal{W}_{mech} - \nabla_{n+1} \cdot \mathbf{q}, \quad \text{in} \quad B_{n+1}
\] (2.49)

where \( \mathcal{W}_{mech} \) is the mechanical dissipation and \( \mathbf{q} \) is the heat flux. The isotropic constitutive equation for the heat flux \( \mathbf{q} \) is given by Fourier’s law as follows:

\[
\mathbf{q} = -K \nabla_{n+1} \theta
\] (2.50)
where the conductivity $K(\theta) \geq 0$. The mechanical dissipation, $W_{\text{mech}}$, is specified in terms of the plastic power by the following empirical law

$$W_{\text{mech}} = \omega \mathbf{T} \cdot \mathbf{D}^p = \omega (1 - f) \sigma_m \dot{\epsilon}^p$$  \hspace{1cm} (2.51)

where $\omega \in [0.85, 0.95]$ is a constant dissipation factor that represents the fraction of the plastic work that is dissipated as heat. In this work, the non-dissipative latent heating is considered negligible in comparison to the mechanical dissipation $W_{\text{mech}}$.

Let $\vartheta$ represent an admissible temperature field expressed over $\mathcal{B}_n$. A variational form of the time discrete equation can be expressed as

$$G^\text{ther}(\theta_{n+1}, \vartheta) = \int_{\mathcal{B}_{n+1}} \frac{\rho c}{\Delta t} (\theta_{n+1} - \theta_n) \, \vartheta \, dV + \int_{\mathcal{B}_{n+1}} K(\nabla n+1 \theta_{n+1}) \cdot (\nabla n+1 \vartheta) \, dV - \int_{\partial \mathcal{B}_{n+1}} W_{\text{mech},n+1} \vartheta \, dV - \int_{\partial \mathcal{B}_{n+1}} q_n \, dA = 0$$  \hspace{1cm} (2.52)

Here $q_n$ refers to the outward normal heat flux. The following forms of thermal boundary conditions (b.c’s) have been considered in this work:

$$q_n = q_0 \quad \text{Neumann b.c.} \hspace{1cm} (2.53)$$

$$q_n = h_0 (\theta - \theta_\infty) \quad \text{Convective b.c.} \hspace{1cm} (2.54)$$

$$q_n = h_c (\theta - \theta_d) - w * q_f \quad \text{Contact b.c.} \hspace{1cm} (2.55)$$

$$q_n = \epsilon (\theta^4 - \theta^4_\infty) \quad \text{Radiation b.c.} \hspace{1cm} (2.56)$$

where $h_0$ is the heat transfer coefficient in the non-contact region, $h_c$ is the heat transfer coefficient in the contact region, $\theta_d$ refers to the die temperature, $\theta_\infty$ is the ambient temperature, $\epsilon$ is the Stefan-Boltzmann constant and $w$ is a factor denoting the distribution of frictional heat (taken as $w = 0.75$, based on [52, 53]). Further, $q_f$ is the heat generated through friction, and calculated by,

$$q_f = |\mathbf{\lambda}_t \cdot \mathbf{v}_n|$$  \hspace{1cm} (2.57)
where $\lambda_t$ is the tangential traction and $v_n$ is the slip velocity. The tractions $\lambda$ at time $t_{n+1}$ are computed in the contact sub-problem. A complete linearization of the above weak form (Equation (2.52)) was performed as part of the direct thermal analysis and the solution methodology is described extensively in [54].

### 2.5 The coupled solution

A two level iterative scheme is employed at each increment to solve the field equations governing the conservation of linear momentum (mechanical step) followed by the conservation of energy in the workpiece (thermal step). Each iterative step involves the solution of a non-linear deformation problem at fixed (predicted) temperature of the workpiece [Phase I], followed by a heat conduction problem in the workpiece for a fixed (predicted) body configuration [Phase II]. The implementation was carried out in a completely object oriented environment. These computational features of the present simulator will not be discussed here and details can be found in [38, 40, 54, 55].

### 2.6 Simulating material response, during thermomechanical processing, through the developed phenomenological approach

In this section, examples demonstrate the performance of the proposed computational framework for porous media, materials with explicit microstructural parameters during hot forming processes. These examples also provide the motivation for the control and design problems to be discussed in later chapters. The mate-
rial properties of the workpiece are described as necessary in the examples. Additional representative examples validating the outlined procedure are presented in [50, 51, 54, 55].

2.6.1 Example 1: Axisymmetric upsetting of a porous billet

This example is concerned with the simulation of axisymmetric upsetting and has been used as a benchmark problem in the isothermal case [49]. The billet is cylindrical, with an initial radius of 1.0 mm and initial height of 3.0 mm. Only one-quarter of the specimen is modelled because of symmetry. A Coulomb friction coefficient of 0.1 is assumed at the interface between the die and workpiece. An upsetting process is carried out until a reduction of 33.34% is obtained. This is carried out at a nominal strain rate of 0.01 s$^{-1}$. The process was studied for a workpiece made of 2024-T351 Aluminum alloy with an initial void fraction of $f_o = 5\%$ and at an initial temperature of 300K. The flow and hardening functions proposed by Lindholm and Johnson are obtained from [78] and are detailed in Appendix A.1. Figures 2.3-2.6 show the initial and the deformed mesh and variation of the direct parameters at time $t = 50$ s.

The large plastic deformation causes self heating of the specimen primarily induced by plastic dissipation. A significant temperature rise (88 K) is observed as a result of plastic work being dissipated as heat. Negligible temperature rise is observed in the dead metal zone. Finally, the variation of the shear modulus $\mu$ in the final forged product as a result of temperature and void fraction evolution is also shown in Figure 2.6. A maximum variation of about 8%, in the shear modulus $\mu$, from the initial value, was observed in the deformed configuration.
Figure 2.3: Representation of the initial and final meshes for the flat die forging process (Example 1).

Figure 2.4: Spatial variation of the scalar state variable and the equivalent stress of the matrix at $t = 50$ s (Example 1).

Figure 2.5: Spatial variation of the temperature and void fraction at $t = 50$ s (Example 1).
2.6.2 Example 2: Verification of direct analysis for processes involving dynamic recrystallization and normal grain growth

A simulation is performed to obtain the uniaxial stress-strain response of 0.2\% C–Steel at different strain rates. These strain rates were chosen from [4], so that the predicted responses can be compared with the reported experimental results. The particular constitutive models and material properties are detailed in Appendix A.2. The strain rates of interest are taken to be $2.8 \times 10^{-4}$, $4.5 \times 10^{-3}$, $1.8 \times 10^{-2}$ and 0.15 sec$^{-1}$. The experimentally observed grain sizes as well as the predicted grain sizes are summarized in Table 2.1. In addition to the evolution of the mean grain size, the stress-strain response is also shown in Figure 2.7. The proposed theory predicts a rapid decrease in mean grain size following the onset of primary recrystallization for the higher strain rates, as has been observed experimentally. In addition, a good agreement of the steady state values of the grain size is observed for these strain rates. It is, though, observed that the model prediction for low strain rates is not accurate. One plausible reason for such behavior is that the mean grain size does not attain a quasi-steady state value towards the end of primary
Table 2.1: Measured and predicted mean grain sizes (in microns) for 0.2% C steel (cast).

<table>
<thead>
<tr>
<th>Strain rate (sec$^{-1}$)</th>
<th>0.2 % C steel</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Measured</td>
<td>Predicted</td>
</tr>
<tr>
<td>0.15</td>
<td>45.8</td>
<td>40.2</td>
</tr>
<tr>
<td>$1.8 \times 10^{-2}$</td>
<td>51.9</td>
<td>47.7</td>
</tr>
<tr>
<td>$4.5 \times 10^{-3}$</td>
<td>55.9</td>
<td>57.1</td>
</tr>
<tr>
<td>$2.8 \times 10^{-4}$</td>
<td>56.2</td>
<td>102.1</td>
</tr>
</tbody>
</table>

Recrystallization (involves multiple peak recrystallization according to [4]). In other words, recrystallization is much lower than grain growth when it should have been the other way around.

### 2.6.3 Example 3: Motivating the need for design in porous materials

The influence of initial product quality and geometry on macroscopic deformation characteristics is demonstrated in this practical application of axisymmetric isothermal closed die forging of a Fe-2 % Si cylindrical workpiece. This example involves the axisymmetric closed die forging operation of a circular billet of exact volume as the die cavity. The billet has a height 5.0 mm and radius 6.315 mm. A stroke of 3.0 mm results in the desired final product. The die profile (i.e. $(r(\eta), z(\eta))$) is
Figure 2.7: The predicted evolution of the mean grain size and the material response in uniaxial tension at various strain rates (Example 2).

described as:

\[
\begin{align*}
\text{shape}(\eta) &= \begin{cases} 
7.6 \times (1 - \eta) \\
818.46 \times \eta^3 - 416.23 \times \eta^2 + 70.55 \times \eta + 3.0 & \text{if } \eta \in [0, 0.1695] \\
15.05 - 79.36 \times \eta + 295.86 \times \eta^2 - 511.87 \times \eta^3 + 403.38 \times \eta^4 - 118.05 \times \eta^5 & \text{if } \eta \in [0.1695, 0.3666] \\
15 & \text{if } \eta \in [0.3666, 1]
\end{cases}
\end{align*}
\]

where \( \eta \in [0, 1] \). The workpiece material is taken to be at an initial temperature of 1273K. The material has a constitutive behavior defined in Appendix A.3. The values of the various mechanical and thermal parameters are also given in Appendix A.3. The friction coefficient is taken to be 0.1. The initial void fraction is assumed to be uniform and equal to 5%. Figure 2.8 shows the quarter geometry of the initial and final configurations. It can be seen, from Figure 2.8, that the finished product does not fill the die cavity even though the workpiece had the same initial volume as the cavity. The location and the volume of the unfilled cavity were observed to
Figure 2.8: Initial guess preform shape and the final product using this guess (Example 3).

vary when the initial conditions (porosity and dimensions of the billet) were changed [59]. Thus, in subsequent chapters, a suitable design methodology will be proposed to identify the initial conditions (say for example, the initial volume) so that the cavity is completely filled. In addition, varying initial conditions were also shown to have a severe effect on the force-stroke characteristics of such processes [40]. Such a dependency of the deformation response and final product quality on the initial preform shape and material properties needs to be accurately studied in order to improve existing metal forming practices.
Chapter 3

Development of an optimization framework - Phenomenological approach

Control of deformation and thermal processes for desired material properties is a significant challenge. An accurate and efficient methodology to control thermo-mechanical processes will have tremendous industrial significance. In the approach developed here, the control problems are posed as optimization problems and a gradient based methodology is developed to design the optimal solution. A basic requirement of any design methodology is an accurate description of the deformation mechanisms involved in the process. The direct deformation forming analysis, developed in Chapter 2, meets this design requirement. However, an efficient design methodology also necessitates the accurate computation of the design derivatives of various deformation related parameters involved in the definition of a related optimization problem. The continuum sensitivity analysis formulated in this chapter provides this significant piece of information. Thus the developments in this
chapter contribute to bridging the gap between deformation process modeling and deformation process optimization. Some of the salient features of this development are itemized below.

- Mathematically accurate description and efficient computation of design derivatives of deformation and temperature related Lagrangian continuum fields.

- Extending continuum sensitivity analysis to compute the sensitivities of various state parameters in the constitutive problem.

- A multi-length scale motivated continuum sensitivity analysis - extending polycrystalline plasticity towards control of deformation problems (Chapter 5).

For convenience, the continuum sensitivity method will be abbreviated by CSM and this convention is utilized in the following sections.

### 3.1 Definition of shape and parameter sensitivities

In this section, the shape and parameter sensitivities of a field Φ, expressed in an updated Lagrangian (UL) framework, are briefly described. Sensitivities of the deformation and material state are quantitative measures of changes in the deformation and material state, respectively, as a result of infinitesimal perturbations to process parameters \( \beta_p \) (parameter sensitivity) or variables that define the initial preform shape \( \beta_s \) (shape sensitivity) [35]. Typical process parameters include the ram speed history, the die surface and the initial material state among others. Figure 3.1 presents a schematic that shows the variation of various fields induced by a variation
in a process parameter. Even though an updated Lagrangian analysis is considered here, a similar representation can be introduced for the total Lagrangian (TL) formulation with \( B_0 \) as the corresponding reference configuration. The variables \( Q \), shown in Figure 3.1, denote the set of material state variables necessary to define the material state and plastic deformation of the workpiece (e.g. \( Q = \{ F^e, s, f, T \} \)).

The generic field \( \Phi \) can represent \( x, Q \) or any other material or deformation related field. The dependence of the UL field \( \Phi = \hat{\Phi}(x, t) \) on \( \beta_p \) can be expressed as follows:

\[
\Phi = \hat{\Phi}(x, t; \beta_p) = \hat{\Phi}(\bar{x}(X, t; \beta_p), t; \beta_p) = \hat{\Phi}(X, t; \beta_p) \tag{3.1}
\]

where the position \( x_n \) is referred to the reference configuration. The parameter sensitivity \( \hat{o} \Phi = \hat{\Phi}(x, t; \beta_p, \Delta\beta_p) \) is defined as the total Gateaux differential [56] of \( \Phi = \hat{\Phi}(x, t; \beta_p) \) in the direction \( \Delta\beta_p \) computed at \( \beta_p \):

\[
\hat{o} \Phi(x, t; \beta_p, \Delta\beta_p) = \hat{o} \Phi(X, t; \beta_p, \Delta\beta_p) = \frac{d}{d\lambda} \hat{\Phi}(X, t; \beta_p + \lambda\Delta\beta_p) \bigg|_{\lambda=0} \tag{3.2}
\]

The parameter sensitivity \( \hat{o} \Phi \) can be approximated as the difference between two values of the field \( \Phi \), that result due to two different forming processes defined by the parameters \( \beta_p + \Delta\beta_p \) and \( \beta_p \) (Figure 3.1), i.e.

\[
\hat{o} \Phi(x, t; \beta_p, \Delta\beta_p) = \\
\hat{\Phi}(\bar{x}(X, t; \beta_p + \Delta\beta_p), t; \beta_p + \Delta\beta_p) - \hat{\Phi}(\bar{x}(X, t; \beta_p), t; \beta_p) = \\
\hat{\Phi}(X, t; \beta_p + \Delta\beta_p) - \hat{\Phi}(X, t; \beta_p) \tag{3.3}
\]

For shape sensitivity analysis, consider Figure 3.2. A design independent reference material configuration \( B_R \) is introduced and a smooth one-to-one design dependent geometric mapping defined on \( B_R \) results in an initial configuration \( B_0 \). The geo-
Figure 3.1: Schematic definition of the parameter sensitivities in the time increment \([t_n, t_{n+1}]\) using an UL sensitivity formulation. \(B_n\), \(n = 1, 2, \ldots\), refer to the configurations that the workpiece occupies at various times during the deformation process defined by setting the process parameters to the value \(\beta_p\) (reference problem), whereas \(B'_n\), \(n = 1, 2, \ldots\), refer to the configurations resulting from the same deformation process but with process parameters set to \(\beta_p + \Delta \beta_p\) (perturbed problem). The preform \(B_0\) remains the same in both reference and perturbed problems.
Figure 3.2: Schematic definition of the shape sensitivities in the time increment $[t_n, t_{n+1}]$ using an UL sensitivity formulation. $B_n$, $n = 1, 2, \ldots$, refer to the configurations that the workpiece occupies at various times in a given deformation process for a preform $B_0$ defined by the shape parameters set to the value $\beta_s$ (reference problem), whereas $B'_n$, $n = 1, 2, \ldots$, refer to the perturbed configurations resulting from the same deformation process but with a preform $B'_0$ defined by the shape parameters $\beta_s + \Delta \beta_s$ (perturbed problem). The process parameters (die surface, ram speed, etc.) remain the same in both reference and perturbed problems.
metric mapping which defines \( \mathcal{B}_0 \) is described as

\[
X = \bar{X}(Y; \beta_s) \quad \forall Y \in \mathcal{B}_R
\]  
(3.4)

Note that the initial configuration \( \mathcal{B}_0 \) varies with the perturbations \( \Delta \beta_s \). Therefore one needs to follow the variation of the field for each given particle \( Y \) defined in the configuration \( \mathcal{B}_R \), before evaluating the shape derivatives of a field. It is from this configuration that all preforms are obtained via the deformation gradient \( F_R \). The dependence of the field \( \Phi = \hat{\Phi}(x_n, t) \) on \( \beta_s \) can thus be expressed as:

\[
\Phi = \hat{\Phi}(x_n, t; \beta_s) = \Phi(X, t; \beta_s) = \bar{\Phi}(Y, t; \beta_s)
\]  
(3.5)

The shape sensitivity \( \hat{\Phi} = \hat{\Phi}(x_n, t; \beta_s, \Delta \beta_s) \) is then defined as the total Gateaux differential of \( \Phi = \hat{\Phi}(x_n, t; \beta_s) \) in the direction \( \Delta \beta_s \) computed at \( \beta_s \)

\[
\hat{\Phi}(x_n, t; \beta_s, \Delta \beta_s) = \hat{\Phi}(X, t; \beta_s, \Delta \beta_s) = \hat{\Phi}(Y, t; \beta_s, \Delta \beta_s)
\]

\[
= \frac{d}{d\lambda} \Phi(Y, t; \beta_s + \lambda \Delta \beta_s) \bigg|_{\lambda=0}
\]  
(3.6)

Similar to the parameter sensitivity, the shape sensitivity \( \hat{\Phi} \) can also be approximated as the difference between two values of the field \( \Phi \), that result due to two different initial configurations defined by the shape parameters \( \beta_s + \Delta \beta_s \) and \( \beta_s \), i.e.

\[
\hat{\Phi}(x_n, t; \beta_s, \Delta \beta_s) =
\]

\[
\hat{\Phi}(x_n, t; \beta_s + \Delta \beta_s, t; \beta_s + \Delta \beta_s) - \hat{\Phi}(x_n, t; \beta_s, \beta_s) + O(\|\Delta \beta_s\|^2) =
\]

\[
\hat{\Phi}(X; \beta_s + \Delta \beta_s, t; \beta_s + \Delta \beta_s) - \hat{\Phi}(X; \beta_s, \beta_s) =
\]

\[
\hat{\Phi}(Y; \beta_s + \Delta \beta_s, t; \beta_s) - \hat{\Phi}(Y; \beta_s, \beta_s)
\]  
(3.7)

Note that once the shape differentiation in Equation (3.7) has been performed, one can set \( F_R = I \). It is then the perturbation \( \hat{F}_R \) (or equivalently the velocity design
gradient $L_0 \equiv F_R^\circ F_R^{-1}$) that drives the subsequent calculation of shape sensitivities.

To simplify the presentation, the same notation $\circ$ is used to define both parameter and shape sensitivities, but the reader should keep in mind the fundamental difference between these two terms as defined in Equations (3.2) and (3.6), respectively.

The above definitions can be applied to both total and updated Lagrangian framework with the appropriate choice of the reference configuration. At this point, the interested reader is referred to [51] for additional details on the TL, UL sensitivity formulations and the sensitivity analysis in the context of multi-stage processing.

**Remark 1:** It is interesting that in an UL framework, one can treat parameter and shape sensitivity problems in a unified way. For an UL framework, the differences between parameter and shape sensitivity analysis are introduced in the initial conditions. It is further true that within an UL framework the sensitivity analysis of multi-stage deformation processes (with different design variables for each stage) retains a mathematical structure identical to that of the sensitivity analysis of single-stage processes. This issue is extensively discussed in [51].

### 3.2 Sensitivity kinematic problem

In this section, the equations governing the sensitivity fields are computed at the continuum level. The sensitivity of the equilibrium equation is directly considered so as to establish a principle of virtual work like equation for the calculation of the sensitivity of deformation fields [40, 41]. Consistent with the above analysis, the sensitivity constitutive and sensitivity thermal equations are derived from the corresponding continuum equations rather than their numerically integrated counterparts. The sensitivity deformation problem is developed on the reference con-
figuration $\mathcal{B}_n$ (in an UL framework). The design differentiation of the equilibrium equation (Equation (2.8)) results in the following:

$$\nabla_n^\circ \mathbf{P} + \mathbf{f} = 0, \ \forall \ t \in [t_n, t_{n+1}] \quad (3.8)$$

A variational form for the sensitivity equilibrium equation can be posed as follows:

Calculate $\hat{x} = \hat{x}(x_n, t; \beta, \Delta \beta)$ such that

$$\int_{\mathcal{B}_n} \hat{P} \cdot \nabla_n \hat{\eta} \, dV_n - \int_{\mathcal{B}_n} \mathbf{P} \left[ \nabla_n \cdot \mathbf{L}_n^T \right] \cdot \hat{\eta} \, dV_n - \int_{\mathcal{B}_n} \left( \mathbf{P} \mathbf{L}_n^T \cdot \nabla_n \hat{\eta} \right) \, dV_n =$$

$$\int_{\Gamma_n} \left\{ \lambda - \left[ \mathbf{L}_n \cdot (\mathbf{N}_n \otimes \mathbf{N}_n) \right] \lambda \right\} \cdot \hat{\eta} \, dA_n \quad (3.9)$$

for every $\hat{\eta}$, where $\hat{\eta}$ is a kinematically admissible sensitivity deformation field expressed over the reference configuration $\mathcal{B}_n$. Also, $\beta$ is the design vector (can represent either $\beta_p$ or $\beta_s$), $\Delta \beta$ represents a perturbation to the design vector, $\mathbf{N}_n$ is the unit normal in $\Gamma_n$ and $\mathbf{L}_n \equiv \nabla_n^\circ \hat{x}(x_n, t; \beta, \Delta \beta) = \hat{\mathbf{F}}_n \hat{\mathbf{F}}^{-1}_n$ refers to the design velocity gradient. In the case of parameter sensitivity analysis, the design velocity gradient at time $t_0$, $\mathbf{L}_0 = \mathbf{0}$. In the case of shape sensitivity analysis, the design velocity gradient at time $t_0$, $\mathbf{L}_0 = \nabla_0^\circ \mathbf{x}(\mathbf{x}; \beta_s, \Delta \beta_s) = \hat{\mathbf{F}}_R \hat{\mathbf{F}}^{-1}_R$. The solution of this variational sensitivity problem involves evaluating the key relationships between $\hat{\mathbf{P}}$ and $\left[ \hat{\mathbf{x}}, \hat{\theta} \right]$ which is part of the constitutive sensitivity problem and between $\hat{\lambda}$ and $\hat{\mathbf{x}}$, which is described by the sensitivity contact problem.

The relationship between $\hat{\mathbf{P}}$ and $\left[ \hat{\mathbf{x}}, \hat{\theta} \right]$ is linear and is denoted as follows:

$$\hat{\mathbf{P}} = \mathbf{A} \left[ \mathbf{F} \right] + \mathbf{C} \hat{\theta} + \mathbf{B} \quad (3.10)$$

where $\mathbf{A}$ is a fourth order tensor and $\mathbf{B}, \mathbf{C}$ are second order tensors, to be evaluated. These tensors will be shown to be constants, defined from known direct fields at the current time and sensitivity fields at the previous time step. The relationship
between $\tilde{\lambda}$ and $\tilde{x}$ is non-trivial and obtained from the sensitivity contact problem as [40]:

$$
\tilde{\lambda} = D \left[ \tilde{x} \right] + d
$$

(3.11)

where $D$ is a second order tensor and $d$ a vector.

### 3.3 Sensitivity constitutive problem

In this constitutive sensitivity problem, the relationship between $\tilde{T}$ and $\left[ \tilde{F}_{n+1}, \tilde{\theta}_{n+1} \right]$, as required by the solution of the sensitivity thermo-mechanical problem, is computed. The sensitivity constitutive problem discussed below is specific for a porous medium. Development of sensitivity problems for other materials follows on similar lines and has been detailed elsewhere [50, 54]. As part of the update procedure, one computes the set $\left\{ \tilde{T}, \tilde{s}, \tilde{f}, \tilde{F}^e \right\}$ at the end of the time increment $t_{n+1}$ when the sensitivity of the total deformation gradient $\tilde{F}_{n+1}$ and the sensitivity of the temperature field $\tilde{\theta}_{n+1}$ are given. The sensitivity of the mechanical dissipation $\tilde{W}_{\text{mech}}$ is also computed as it is part of the driving force for the thermal sensitivity problem at time $t_{n+1}$ [54]. In addition, the solution of the direct thermo-mechanical problem is known at time $t_{n+1}$ i.e. the set $\{ T, s, f, F^e \}$, the body configuration $B_{n+1}$ as well as the temperature field $\theta_{n+1}$ are known at $t_{n+1}$ (from Chapter 2). Due to non-linear material response, the sensitivity constitutive problem is history dependent and the solution of the sensitivity problem at time $t_{n+1}$ is assumed known, yielding the variables $\left\{ \tilde{T}, \tilde{s}, \tilde{f}, \tilde{F}^e \right\}$ at the beginning of the time increment ($t = t_n$). It will be shown later (Equation (3.45)) that the deformation sensitivity response does not explicitly depend on the history of the temperature sensitivity but is dependent only on the instantaneous temperature sensitivity response $\tilde{\theta}_{n+1}$. The solution of
the sensitivity sub-problem is advanced within the incremental solution scheme by integrating the evolution equations for the sensitivity of the plastic and thermal deformation gradients, the evolution equation for the sensitivity of the state variable $s$ and the void fraction $f$. As part of this sub-problem, the linear relationship between $\bar{T}$ and $\{\bar{F}, \bar{\theta}\}$ at time $t_{n+1}$ is also computed. This relationship is then be used to compute the constants $\mathbf{A}, \mathbf{B}$ and $\mathbf{C}$, in Equation (3.10), as needed in the solution of the sensitivity thermo-mechanical problem (Equation (3.9)).

### 3.3.1 Computing the linear relation between $\bar{F}_{n+1}^p$ and $\{\bar{F}_{n+1}^{e}, \bar{\theta}_{n+1}\}$

The evolution equation for $\bar{F}^p$ is given as, $\dot{\bar{F}}^p F^p - 1 = \bar{D}^p$, assuming that the plastic spin $\bar{W}^p = 0$. Consider the design differentiation of this evolution equation. It is clear that $\bar{F}^p$ is completely specified by the sensitivity of the plastic stretching rate, $\bar{D}^p$ (again drop the subscript $(n + 1)$ for convenience):

$$\frac{\partial \bar{F}^p}{\partial t} = \bar{D}^p \bar{F}^p + \bar{D}^p F^p \quad (3.12)$$

$\bar{D}^p$ can be computed by design-differentiation of the flow rule (Equation (2.17)) as,

$$\bar{D}^p = (\dot{\gamma} \frac{\partial}{\partial T} \Phi) = \dot{\gamma} \left[ (\partial_S \Phi) N - \frac{1}{3} (\partial_p \Phi) I \right] \quad (3.13)$$

which can be written as follows:

$$\bar{D}^p = D_1 \bar{\sigma}_m + D_2 \bar{f} + D_3 \bar{p} + D_4 \bar{S} + D_5 \bar{s} + D_6 \bar{\theta} + d_7 \bar{T}' \quad (3.14)$$

where $D_1$, $D_2$, $D_3$, $D_4$, $D_5$, $D_6$ are constant second order tensors, $d_7$ a known scalar and $\bar{T}'$ is the deviatoric part of the sensitivity of the rotation neutralized Cauchy stress, $\bar{T}$. These constants depend on the choice of the material response
function for the flow rule. For a constitutive model that incorporates damage (as in Chapter 2), the constants can be evaluated as:

\[
\begin{align*}
D_1 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{\sigma m} N - \frac{1}{3} \Phi_{p m} I \right\} \\
D_2 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{f} N - \frac{1}{3} \Phi_{p f} I \right\} \\
D_3 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{p} N - \frac{1}{3} \Phi_{p p} I \right\} \\
D_4 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{SS} N - \frac{\Phi_{S}}{S} N - \frac{1}{3} \Phi_{p s} I \right\} \\
D_5 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{S} N - \frac{1}{3} \Phi_{p s} I \right\} \\
D_6 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{S} N - \frac{1}{3} \Phi_{p S} I \right\} \\
D_7 &= \frac{\dot{\gamma}}{\dot{\gamma}} \bar{D}^p + \dot{\gamma} \left\{ \Phi_{S} N - \frac{1}{3} \Phi_{p S} I \right\} \\
d_7 &= \frac{\dot{\gamma}}{\dot{\gamma}} \frac{\Phi_{S}}{S}
\end{align*}
\]

where \( \Phi \) is the potential function, \( N \) is the normal obtained from the stress deviator, \( \Phi_{S} \equiv \partial_{S} \Phi \) and \( \Phi_{p} \equiv \partial_{p} \Phi \) and subscripts denote partial derivatives. Other evaluations, including the ones incorporating grain size effects, are detailed in [50, 51].

From Equation (3.14), \( \bar{D}^{p} \) can be expressed in terms of \( \bar{p}, \bar{S}, \bar{\theta} \) and \( \bar{T}^{p} \) if \( \bar{\sigma}_{m}, \bar{f}, \bar{s} \) can be expressed in terms of \( \bar{p}, \bar{S}, \bar{\theta} \). Indeed, design-differentiate the consistency condition (Equation (2.10)) to derive the following:

\[
\bar{\Phi} = \Phi(\bar{\sigma}_{m}, \bar{f}, \bar{p}, \bar{S}) = 0
\]

where \( \bar{\Phi} \) is expressed in terms of \( \bar{\sigma}_{m}, \bar{f}, \bar{p}, \bar{S} \) and \( \bar{s} \) by taking partial derivatives of \( \Phi \) with respect to its arguments. The resulting equation takes the following form:

\[
c_1 \bar{\sigma}_{m} + c_2 \bar{f} + c_3 \bar{s} = c_5 \bar{p} + c_6 \bar{S} + c_7 \bar{\theta}
\]

where the constants \( c_1, \ldots, c_7 \) can be easily evaluated. Note that for this particular GTN (Gurson-Tvergaard-Needleman) model selected, \( c_3 = c_7 = 0 \). The evolution
equation for the sensitivities $\ddot{f}$ and $\ddot{s}$ can be evaluated from their direct counterparts (Equations (2.16) and (2.21)) as:

$$\frac{\partial \ddot{f}}{\partial t} = -\ddot{f} \text{tr} \ddot{D}^p + (1 - \ddot{f}) \text{tr} \dddot{D}^p$$

(3.25)

$$\frac{\partial \ddot{s}}{\partial t} = g_{\sigma_m} \sigma_m + g_s \ddot{s} + g_{\theta} \ddot{\theta}$$

(3.26)

where $g$ is the hardening function and $\text{tr} \dddot{D}^p = -\dddot{\gamma} \partial_p \Phi$. An Euler-backward time integration scheme applied to the evolution equations for the state variables (Equations (3.25) and (3.26)) result in the following:

$$b_1 \ddot{\sigma}_m + b_2 \ddot{f} + b_3 \ddot{s} = b_4 + b_5 \dddot{p} + b_6 \dddot{S} + b_7 \dddot{\theta}$$

(3.27)

$$a_1 \ddot{\sigma}_m + a_2 \ddot{s} = a_3 + a_4 \dddot{\theta}$$

(3.28)

where the constants $a_1, \ldots, a_4, b_1, \ldots, b_7$ are computed as part of the solution process.

Equations (3.24), (3.27) and (3.28) can be solved to yield the following:

$$\begin{pmatrix}
\ddot{\sigma}_m \\
\ddot{f} \\
\ddot{s}
\end{pmatrix} = \begin{pmatrix}
M_{11} & M_{12} & M_{13} \\
M_{21} & M_{22} & M_{23} \\
M_{31} & M_{32} & M_{33}
\end{pmatrix} \begin{pmatrix}
\dddot{p} \\
\dddot{S} \\
\dddot{\theta}
\end{pmatrix} + \begin{pmatrix}
m_1 \\
m_2 \\
m_3
\end{pmatrix}$$

(3.29)

where the $3 \times 3$ matrix $M$ and the scalars $m_1, m_2, m_3$ are constants. Using the above solution for $\ddot{\sigma}_m, \ddot{f}$ and $\ddot{s}$ in terms of $\dddot{p}, \dddot{S}$ and $\dddot{\theta}$ in Equation (3.14), one can relate $\ddot{D}^p$ to $\dddot{p}, \dddot{S}, \dddot{\theta}$ and $\dddot{T}$. Let this relation be expressed as:

$$\ddot{D}^p = D_1^p \dddot{p} + D_2^p \dddot{S} + D_3^p \dddot{\theta} + D_4^p + d_r \dddot{T}$$

(3.30)

where $D_1^p, D_2^p, D_3^p, D_4^p$ are known second order tensors and $d_r$, a scalar, defined earlier. The dependence of $\dddot{T}$ on $\dddot{F}^e$ is derived by design-differentiation of the hyperelastic model of Equation (2.5) as:

$$\dddot{T} = \mathcal{L}^e [\dddot{E}^e] + \ddot{\mathcal{L}}^e [\dddot{E}^e]$$

(3.31)
\[ \mathcal{L}^e = 2 \mu \mathbf{I} + \left( \kappa - \frac{2}{3} \mu \right) \mathbf{I} \otimes \mathbf{I} \]  \hspace{1cm} (3.32)

Here \( \mu \) and \( \kappa \) are assumed to be functions of \( [\theta, f] \) as in Chapter 2. It is also known, from [36], that:

\[
\mathbf{E}^e = 4(\mathbf{U}^e + \mathbf{I})^{-1} \mathbf{U}^e (\mathbf{U}^e + \mathbf{I})^{-1} \]  \hspace{1cm} (3.33)

\[
\mathbf{U}^e = \text{sym} \left\{ (\mathbf{U}^e)^{-1} \text{sym} \left( (\mathbf{F}^e)^T \mathbf{F}^e \right) \right\} \]  \hspace{1cm} (3.34)

where \( \mathbf{U}^e \) is the stretch tensor obtained through the polar decomposition of the elastic part of deformation gradient, \( \mathbf{F}^e \). The second term on the RHS of Equation (3.31) results in a linear relation of \( \mathbf{T}^e \) with \( \mathbf{f} \) and \( \mathbf{\theta} \). Using the second equation in the linear system in Equation (3.29), one can substitute \( \mathbf{f} \) in terms of \( \mathbf{p}, \mathbf{S} \) and \( \mathbf{\theta} \). The following relation between \( \mathbf{T}'^e \) and the set \( \{\mathbf{F}^e, \mathbf{p}, \mathbf{S}, \mathbf{\theta}\} \) is then obtained:

\[
\mathbf{T}'^e = E_1 \mathbf{p} + E_2 \mathbf{S} + E_3 \mathbf{\theta} + E_4 + E_5 \left[ \mathbf{F}^e \right] \]  \hspace{1cm} (3.35)

where \( E_1, E_2, E_3, E_4 \) are known second order tensors and \( E_5 \) a known fourth order tensor. Using Equation (3.35), Equation (3.30) can be simplified to:

\[
\mathbf{D}^p = D_1'' \mathbf{p} + D_2'' \mathbf{S} + D_3'' \mathbf{\theta} + D_4'' + D_5'' \left[ \mathbf{F}^e \right] \]  \hspace{1cm} (3.36)

where \( D_1'', D_2'', D_3'', D_4'' \) are known second order tensors and \( D_5'' = d_7 E_5 \).

The sensitivities \( \mathbf{S} \) and \( \mathbf{p} \), are evaluated from their direct counterparts (Equations (2.11) and (2.12)) as follows:

\[
\mathbf{S} = \left( \mathbf{T}' \cdot \mathbf{T}' \right)^{\circ} = \frac{1}{S} \mathbf{T}' \cdot \mathbf{T}' \]  \hspace{1cm} (3.37)

\[
\mathbf{p} = -\text{tr} \mathbf{T}'/3 \]  \hspace{1cm} (3.38)

where \( \mathbf{T}' \) is the deviatoric part of the sensitivity of the rotation neutralized Cauchy stress. Substitution of Equation (3.35) in the above equations results in linear
systems that can be solved to compute $\dot{\bar{p}}$ and $\dot{\bar{S}}$ in terms of $\bar{F}^e$ and $\dot{\theta}$. The derived functional form of $\dot{\bar{S}}$ and $\dot{\bar{p}}$ can finally be expressed as follows:

\[
\dot{\bar{S}} = k_{11} + k_{12} \dot{\bar{\theta}} + k_1(\bar{F}^e) \tag{3.39}
\]

\[
\dot{\bar{p}} = k_{21} + k_{22} \dot{\bar{\theta}} + k_2(\bar{F}^e) \tag{3.40}
\]

where $k_{11}$, $k_{12}$, $k_{21}$, $k_{22}$ are known constants and $k_1$ and $k_2$ are known scalar-valued function of a second order tensor, all defined at time $t_{n+1}$. Substitution of these relations in Equation (3.36) results in the following final expression:

\[
\bar{D}^p = \mathcal{A}'[\bar{F}^e] + A_1 \dot{\bar{\theta}} + A_2 \tag{3.41}
\]

$A_1$, $A_2$ are known second order tensors and $\mathcal{A}'$ is a known fourth order tensor defined at $t_{n+1}$. All tensor transformations required for the derivations above can easily be implemented using the equivalent matrix and vector transformations introduced in [40].

An Euler-backward time integration scheme over $(t_n, t_{n+1})$ applied to the evolution equations for the sensitivities of the plastic deformation gradient (Equation (3.12)) yields (subscript $(n+1)$ is included for clarity):

\[
\bar{F}^p_{n+1} (\bar{F}^p_n)^{-1} = \Delta F^p \bar{F}^p_n (\bar{F}^p_n)^{-1} (\Delta F^p)^{-1} + \Delta t \bar{D}^p_{n+1} \tag{3.42}
\]

where,

\[
\Delta F^p = F^p_{n+1} (F^p_n)^{-1} = \exp \left( \Delta t \bar{D}^p_{n+1} \right) \tag{3.43}
\]

with $\Delta t = t_{n+1} - t_n$. Substituting Equation (3.41) in Equation (3.42), one obtains the desired linear relationship between $\bar{F}^p_{n+1}$ and $\{ \bar{F}^e_{n+1}, \dot{\theta}_{n+1} \}$. 

3.3.2 Computing the linear relation between \( \overset{o}{F}_{n+1} \) and \( \left\{ \overset{o}{F}_{n+1}, \overset{o}{\theta}_{n+1} \right\} \)

Starting from the multiplicative decomposition of the deformation gradient (Equation (2.2)), one can write

\[
\overset{o}{F}_{n+1} = \overset{o}{F}_{n+1}^e F_{n+1}^p F_{n+1}^\theta + F_{n+1}^e \overset{o}{F}_{n+1}^p F_{n+1}^\theta + F_{n+1}^e F_{n+1}^p \overset{o}{F}_{n+1}^\theta
\]  
(3.44)

The evolution equation for \( \overset{o}{F}_{n+1}^\theta \) can be derived from the evolution of the thermal deformation gradient given in the direct problem in Equation (2.3) and is expressed as:

\[
\overset{o}{F}_{n+1}^\theta (F_{n+1}^\theta)^{-1} = \beta \overset{o}{\theta}_{n+1} I
\]  
(3.45)

This is derived and discussed in follows [54]. Equation (3.44) can then be simplified as

\[
(F_{n+1}^e)^{-1} (\overset{o}{F}_{n+1} F_{n+1}^{-1}) F_{n+1}^e = (F_{n+1}^e)^{-1} F_{n+1}^e + \overset{o}{F}_{n+1}^p (F_{n+1}^p)^{-1} + \beta \overset{o}{\theta}_{n+1} I
\]  
(3.46)

assuming \( \beta \) is a constant. Substitution of the linear relationship between \( \overset{o}{F}_{n+1}^p \) and \( \left\{ \overset{o}{F}_{n+1}^e, \overset{o}{\theta}_{n+1} \right\} \) (from the previous sub-section) in Equation (3.46) results in the desired linear relationship that can be expressed as:

\[
\overset{o}{F}_{n+1} = \mathcal{B}'(V_{n+1}) \left[ \overset{o}{F}_{n+1} \right] + A_3 \left( V_{n+1}, \overset{o}{V}_n \right) + A_4 \left( V_{n+1}, \overset{o}{\theta}_{n+1} \right) \]  
(3.47)

where \( A_3 \) and \( A_4 \) are known second order tensor functions and \( \mathcal{B}' \), a known fourth order tensor function. The arguments in these functions are here given in terms of the set \( V \equiv [T, s, f, F^p] \) (at time \( t_{n+1} \)) and its sensitivity \( \overset{o}{V} \) (at time \( t_n \)).
3.3.3 Computing the linear relation between

\[ T_{n+1} \text{ and } \{ \overset{\circ}{F}_{n+1}, \overset{\circ}{\theta}_{n+1} \} \]

The relationship between \( T_{n+1} \) and \( \{ \overset{\circ}{F}_{n+1}, \overset{\circ}{\theta}_{n+1} \} \) is developed in [39] by differentiating Equation (2.6). It has been evaluated as:

\[ T = (\det(U^e))^{-1} R^e T R^e T - \text{tr}E^e T + \left\{ R^e R^e T - T R^e R^e T \right\} \]  \hspace{1cm} (3.48)

where

\[ \overset{\circ}{R}^e R^e T = F^e F^{e-1} - R^e \text{sym} \left( U^e \text{sym} \left( F^{e-1} F^e \right) \right) U^{e-1} R^e T \] \hspace{1cm} (3.49)

Substitution of the linear relation between \( \overset{\circ}{F}^e_{n+1} \) and \( \{ \overset{\circ}{F}_{n+1}, \overset{\circ}{\theta}_{n+1} \} \) (Equation (3.47)) in Equation (3.48), results in a linear relation between \( T_{n+1} \) and \( \{ \overset{\circ}{F}_{n+1}, \overset{\circ}{\theta}_{n+1} \} \) that is similar in form to that given in the RHS of Equation (3.47).

3.3.4 Postprocessing operations: Calculation of \( \overset{\circ}{F}^e_{n+1} \) and the set \( \{ p_{n+1}, S_{n+1}, \sigma_{m,n+1}, f_{n+1}, s_{n+1} \} \) given \( \{ \overset{\circ}{F}_{n+1}, \overset{\circ}{\theta}_{n+1} \} \)

Many of the above presented linear relations can be used for postprocessing operations once the solution for \( \overset{\circ}{F}_{n+1} \) and \( \overset{\circ}{\theta}_{n+1} \) is complete within a time step. With \( \overset{\circ}{F}^e_{n+1} \) computed from Equation (3.47), one can evaluate \( S_{n+1} \) and \( p_{n+1} \) from Equations (3.39) and (3.40), respectively. Finally, Equation (3.29) can be used to compute \( f_{n+1}, \sigma_{m,n+1} \) and \( s_{n+1} \).

3.3.5 Computing the linear relation between

\( \overset{\circ}{W}_{mech,n+1} \) and \( \{ \overset{\circ}{F}_{n+1}, \overset{\circ}{\theta}_{n+1} \} \)

Using Equation (2.51), \( \overset{\circ}{W}_{mech} \) can be computed as follows:

\[ \overset{\circ}{W}_{mech} = \omega \left[ (1 - f)(\overset{\circ}{\sigma}_m \overset{\circ}{\varepsilon}^p + \sigma_m \overset{\circ}{\varepsilon}^p) - f \sigma_m \overset{\circ}{\varepsilon}^p \right] \] \hspace{1cm} (3.50)
The sensitivity field, $\tilde{\epsilon}^p$, can be easily computed by design differentiation of Equation (2.20) in terms of the sensitivity fields $\hat{\sigma}_m$, $\hat{s}$ and $\hat{\theta}$. Further, using the known linear relation between various quantities (computed in the previous sub-sections), the required linear relation between $\tilde{\epsilon}^p$ and $\{\tilde{F}_{n+1}, \tilde{\theta}_{n+1}\}$ can be obtained. One finally obtains the following expression for $\tilde{W}_{\text{mech}}$ at $t_{n+1}$ as:

$$\tilde{W}_{\text{mech},n+1} = K(V_{n+1}) \cdot \tilde{F}_{n+1} + \tilde{k}_1(V_{n+1}, \tilde{V}_n) + \tilde{k}_2(V_{n+1}) \tilde{\theta}_{n+1}$$  \hspace{1cm} (3.51)

where $K$ is a known second order tensor function and $\tilde{k}_1, \tilde{k}_2$ are known scalar functions.

### 3.4 Thermal sensitivity problem

The thermal sensitivity problem is solved in a similar fashion to the one described in [54]. Note, however, that $\rho c$ and $K$ are functions of the void fraction, $f$ and temperature, $\theta$. The sensitivity thermal evolution equation is obtained by the design differentiation of Equation (2.49):

$$\rho c \frac{\partial \tilde{\theta}}{\partial t} + (\rho c)_f \frac{\partial \tilde{\theta}}{\partial t} + (\rho c)_\theta \frac{\partial \tilde{\theta}}{\partial t} = \tilde{W}_{\text{mech}} - \nabla_{n+1} \cdot \tilde{q}$$  \hspace{1cm} (3.52)

where the subscripts indicate partial derivatives. The spatial divergence of the heat flux can be expressed as:

$$\nabla_{n+1} \cdot \tilde{q} = \nabla_0 \tilde{q} \cdot F_{n+1}^{-T}$$  \hspace{1cm} (3.53)

where the subscripts 0 and $n + 1$ in $\nabla$ denote the design-independent reference configuration, $B_0$ and current configuration, $B_{n+1}$, respectively. Design differentiation of the above equation yields the following:

$$\nabla_{n+1} \cdot \tilde{q} = \nabla_0 \tilde{q} \cdot F_{n+1}^{-T} - \nabla_n \tilde{q} \cdot L_{n+1}^{T} F_{n+1}^{-T}$$  \hspace{1cm} (3.54)
where $L_{n+1} \equiv F_{n+1}^{-1} F_{n+1}$. Design differentiation of Fourier’s first law also yields:

$$
\mathring{q} = -K \nabla_{n+1} \mathring{\theta} - L_{n+1}^T q - K_f \mathring{f} \nabla_{n+1} \mathring{\theta}
$$

(3.55)

Substitution of Equation (3.55) in Equation (3.54) results in the following equation:

$$
\nabla_{n+1} \mathring{\theta} = -\nabla_{n+1} \cdot (K \nabla_{n+1} \mathring{\theta}) - (\nabla_{n+1} \cdot L_{n+1}) \mathring{q} - 2(\nabla_{n+1} q \cdot L_{n+1}) - \nabla_{n+1} \cdot (K_f \mathring{f} \nabla_{n+1} \mathring{\theta})
$$

(3.56)

The thermal sensitivity equation in the workpiece is finally obtained as:

$$
\rho c \frac{\partial \mathring{\theta}}{\partial t} + (\rho c)_{\theta} \frac{\partial \theta}{\partial t} + (\rho c)_f \frac{\partial \mathring{\theta}}{\partial t} = \dot{W}_{mech} + \nabla_{n+1} \cdot (K \nabla_{n+1} \mathring{\theta} + L_{n+1}^T q) + \nabla_{n+1} q \cdot L_{n+1} + \nabla_{n+1} \cdot (K_f \mathring{f} \nabla_{n+1} \mathring{\theta})
$$

(3.57)

An implicit Euler-backward scheme (consistent with the direct analysis) is used to integrate the temperature sensitivity evolution equation. It takes the following form:

$$
\frac{\rho c}{\Delta t} \left( \mathring{\theta}_{n+1} - \mathring{\theta}_n \right) + (\rho c)_\theta \left( \theta_{n+1} - \theta_n \right) \mathring{\theta}_{n+1} + (\rho c)_f \left( \theta_{n+1} - \theta_n \right) \mathring{f}_{n+1} = \dot{W}_{mech,n+1} + \nabla_{n+1} \cdot (K \nabla_{n+1} \mathring{\theta}_{n+1} + L_{n+1}^T q_{n+1}) + \nabla_{n+1} q_{n+1} \cdot L_{n+1} + \nabla_{n+1} \cdot (K_f \mathring{f}_{n+1} \nabla_{n+1} \mathring{\theta})
$$

(3.58)

A weak form of the thermal sensitivity equation posed on the deformed configuration $B_{n+1}$ is now considered. Let $\vartheta$ represent an admissible sensitivity temperature field expressed over $B_{n+1}$. The variational form of Equation (3.58) is posed as:

$$
\int_{B_{n+1}} \frac{\rho c}{\Delta t} \left( \mathring{\theta}_{n+1} - \mathring{\theta}_n \right) \vartheta dV + \int_{B_{n+1}} (\rho c)_\theta \left( \theta_{n+1} - \theta_n \right) \mathring{\theta}_{n+1} \vartheta dV + \int_{B_{n+1}} (\rho c)_f \left( \theta_{n+1} - \theta_n \right) \mathring{f}_{n+1} \vartheta dV = \int_{B_{n+1}} \dot{W}_{mech,n+1} \vartheta dV + \int_{B_{n+1}} \nabla_{n+1} q_{n+1} \cdot \mathring{\theta} dV + \int_{B_{n+1}} \nabla_{n+1} q_{n+1} \cdot \mathring{\theta} dV
$$

(3.59)
The sensitivity thermal boundary conditions are evaluated using Equations (2.53)-(2.56). They take the following forms:

\[^{\circ} q \cdot n = -q \cdot n \]
\text{Neumann b.c.} \quad (3.60)

\[^{\circ} q \cdot n = -q \cdot n + h_0 \, ^{\circ} \theta \]
\text{Convective b.c.} \quad (3.61)

\[^{\circ} q \cdot n = -q \cdot n + h_c (^{\circ} \theta) - w^{\circ} q_f \]
\text{Contact b.c.} \quad (3.62)

\[^{\circ} q \cdot n = -q \cdot n + 4 \, \epsilon \, ^{\circ} \theta^3 \]
\text{Radiation b.c.} \quad (3.63)

where \( h_0, h_c \) are defined in Chapter 2. Note that via the contact regularization assumptions introduced in [39, 41], the regions of the workpiece boundary in contact for the perturbed problem are the same as those computed in the solution of the reference direct problem. Hence, there is no ambiguity in the application of the above conditions for regions in contact. The design differential \( \tilde{n} \) of the unit normal \( n \) to the boundary can be derived as [54]:

\[^{\circ} n = [L \cdot n \otimes n] n - L^T n \]
\quad (3.64)

Finally, the design sensitivity of the frictional dissipation \( q_f \) is evaluated from Equation (2.57) as:

\[^{\circ} q_f = \text{sign}(q_f) \left( \lambda_t \cdot v_n + \lambda_t \cdot \boldsymbol{v}_n \right) \]
\quad (3.65)

Modeling of contact sensitivity and assumed strain sensitivity analysis follows the methodology described in [41] and will not be discussed here.
3.4.1 Initial conditions for the sensitivity constitutive problem

The following set of initial conditions are used in the direct analysis

\[ F^e(X, 0) = I \]
\[ F^p(X, 0) = I \]
\[ s(X, 0) = s_0 \]
\[ f(X, 0) = f_0 \]
\[ \theta(X, 0) = \theta_0 \] (3.66)

The corresponding initial conditions for the sensitivity problem are

\[ \overset{\circ}{F}^e (X, 0) = 0 \]
\[ \overset{\circ}{F}^p (X, 0) = 0 \]
\[ \overset{\circ}{s} (X, 0) = 0 \]
\[ \overset{\circ}{f} (X, 0) = 0 \]
\[ \overset{\circ}{\theta} (X, 0) = 0 \] (3.67)

The boundary conditions for the sensitivity problem are derived from the corresponding boundary conditions of the direct analysis. Some typical non-contact related cases are examined here. For a traction free boundary, \( \overset{\circ}{\lambda} = 0 \). On a boundary where the displacement is prescribed, i.e., where \( x = \bar{x} (X, t) = \bar{x}(X, t) \) with \( \bar{x} \) a design-independent function, one can write \( \overset{\circ}{x} = 0 \). In the case where the ram-speed \( V(t) \) is the design variable, then the sensitivity of the boundary displacement takes the form \( \overset{\circ}{x} = \bar{x}(X, t) = \bar{V} (t) t \), where the sensitivity of the ram speed is given by \( \bar{V} (t) \).
3.5 Validation of sensitivity algorithm

In this section, numerical examples are presented that verify the accuracy of the computed sensitivity fields using the developed sensitivity algorithm (CSM). The computations were performed using Intel processors on the Cornell Theory Center’s AC3 Velocity configuration. In all reported simulations, the a-priori stabilized $F$-bar method with a stabilization parameter $\epsilon = 10^{-04}$ was implemented for 4-noded quadrilateral elements with 4 full integration points and 1 reduced integration point (at the centroid) [41].

3.5.1 Example 4: Validation of shape sensitivity analysis for a porous material

This example is used to validate the algorithm for shape sensitivity analysis in a deformation process where complete dependence of the elastic properties on temperature and void fraction is accounted for. The billet is cylindrical, with an initial radius of 1.0 mm and initial height of 3.0 mm. Only one-quarter of the specimen is modelled because of symmetry. A Coulomb friction coefficient of 0.1 is assumed at the interface between the die and workpiece. An upsetting process is carried out until a reduction of 33.34% is obtained. This is carried out at a nominal strain rate of 0.01 s$^{-1}$. The process was studied for a workpiece made of 2024 − T351 Aluminum alloy with an initial void fraction of $f_o = 5\%$ and an initial temperature of 300K. The flow, hardening functions and material properties are detailed in Appendix A.1. The free surface $R_{\beta}(\alpha)$, of the preform, is represented with a degree 6 Bézier curve (with 7 Bernstein basis functions, see Figure 3.3). Using the restriction $R'_{\beta}(0) = 0$, the representation of $R_{\beta}$ can be defined with 6 independent
Figure 3.3: The free surface in the shape sensitivity analysis of axisymmetric upset forging (Example 4).

design variables $\beta_i$, $i = [1 \ldots 6]$ as follows:

$$R_{\beta}(\alpha) = \sum_{i=1}^{6} \beta_i \phi_i(\alpha)$$

$$Z = 1.5 \alpha \quad 0 \leq \alpha \leq 1$$

(3.68)

where $Z$ represents the axial coordinate, $\alpha$ represents the normalized axial coordinate, $R_{\beta}$ is the radial coordinate and the basis functions are given as

$$\phi_1 = (1.0 - \alpha)^5 (1.0 + 5.0 \alpha)$$

$$\phi_2 = 15.0 \ (1.0 - \alpha)^4 \alpha^2$$

$$\phi_3 = 20.0 \ (1.0 - \alpha)^3 \alpha^3$$

$$\phi_4 = 15.0 \ (1.0 - \alpha)^2 \alpha^4$$

$$\phi_5 = 6.0 \ (1.0 - \alpha) \alpha^5$$

$$\phi_6 = \alpha^6$$

(3.69)

The reference problem was chosen to be defined by $\beta_i = 1.0$ mm, $i = [1 \ldots 6]$, which corresponds to a right circular preform. In this analysis the perturbation to the free surface is through, $\Delta \beta_3 = 10^{-04}$ mm and the forward finite difference computations
Figure 3.4: Representation of the initial and final meshes for the flat die forging process (Example 4).

(FDM) are carried out with a step size of 0.01%. Figures 3.4, 3.5 show the initial configuration, the deformed mesh and variation of the direct parameters at time $t = 50$ s, respectively. Figures 3.6-3.10 show, at $t = 50$ seconds, the variation of the shape sensitivity of the state variable, temperature, void fraction, pressure and shear modulus respectively, using the CSM and FDM sensitivity computations. The FDM and CSM sensitivities are very close to each other.

### 3.5.2 Example 5: Validation of the shape sensitivity analysis for a material undergoing dynamic recrystallization

This section involves the validation of the shape sensitivity analysis for a thermo-mechanical process by a comparison with the forward finite difference method (FDM). Upset forging, as in the previous example, is considered. The material is assumed to be 0.2% C-Steel, whose material properties and constitutive parameters are defined in Appendix A.2. The initial billet was subject to a large height reduction of 33.34% in 500 seconds using a fixed time step of $\Delta t = 1.0$ second at a nominal strain rate of 0.001 $sec^{-1}$. The preform free surface is represented as Equation (3.68). The shape parameters in the reference preform (cylindrical billet) are $\beta_i = 1.0$ mm, $i = [1 \ldots 6]$. Shape sensitivities are taken with respect to the free surface shape which is altered
Figure 3.5: Spatial variation of the scalar state variable, equivalent stress of the matrix, temperature, void fraction, pressure and shear modulus at $t = 50$ s (Example 4).

(a) FDM  
(b) CSM

Figure 3.6: Spatial variation of the shape sensitivity (FDM and CSM) of the scalar state variable at $t = 50$ s (Example 4).
Figure 3.7: Spatial variation of the shape sensitivity (FDM and CSM) of the temperature at $t = 50$ s (Example 4).

Figure 3.8: Spatial variation of the shape sensitivity (FDM and CSM) of the void fraction at $t = 50$ s (Example 4).

Figure 3.9: Spatial variation of the shape sensitivity (FDM and CSM) of the pressure at $t = 50$ s (Example 4).
Figure 3.10: Spatial variation of the shape sensitivity (FDM and CSM) of the shear modulus at $t = 50$ s (Example 4).

by perturbing the design variable $\beta_3$. The coefficient of friction between the die and workpiece is taken as 0.4. Figure 3.11 depicts the distribution of the equivalent stress, equivalent scalar state variable, temperature, mean grain size and the fraction recrystallized in the deformed workpiece at the final time, $t = 500$ s. This solution defines the reference solution at which the sensitivity fields will be computed for a specified perturbation in the design variables.

Figures 3.12-3.14 show, at $t = 500$ seconds, the shape sensitivity of the state variable, temperature and the mean grain size, respectively, using the CSM and FDM sensitivity computations. The FDM sensitivity fields are obtained using the results of the direct analysis and a forward difference approximation for a perturbation of the design variable, $\beta_3$, by $\Delta \beta_3 = 10^{-04}$ mm. These results validate the accuracy proposed continuum shape sensitivity analysis.

### 3.5.3 Example 6: Validation of the thermo-mechanical parameter sensitivity analysis

The objective here is to validate the parameter sensitivity analyses for a thermo-mechanical process by a comparison with the forward finite difference method (FDM).
Figure 3.11: Solution of the reference problem: the spatial variation of the equivalent stress, scalar state variable, temperature and grain size at $t = 500$ s (Example 5).

Figure 3.12: Shape sensitivity of the scalar state variable at $t = 500$ s computed using the FDM and CSM methods (Example 5).
Figure 3.13: Spatial variation of the shape sensitivity of the temperature at $t = 500$ s computed using the FDM and CSM methods (Example 5).

Figure 3.14: Spatial variation of the shape sensitivity of the mean grain size at $t = 500$ s computed using the FDM and CSM methods (Example 5).
The upset forging is considered between parallel flat dies of a cylindrical billet 2 mm in diameter and 3 mm in height. The initial billet was subject to a large height reduction of 33.34% in 50 seconds using a fixed time step of $\Delta t = 1.0$ second. In this parameter sensitivity analysis problem, the ram speed (or the nominal strain rate) is assumed to be the design parameter. Thus parameter sensitivities are taken with respect to the forging rate $V$. The reference forging rate was taken as 0.01 sec$^{-1}$. The perturbation of 1% to this forging velocity was used to drive the sensitivity problems. Thus the perturbation is taken as $\Delta V = 10^{-04}$ sec$^{-1}$.

In addition, the material was chosen to be 1100−Al at an initial temperature of 673K. The coefficient of friction is taken as 0.3. The specific constitutive model and material properties are defined in Appendix A.6. Figure 3.15 depicts the distribution of the equivalent stress, scalar state variable, plastic strain and temperature in the deformed workpiece at $t = 50$ s. This solution defines the reference solution at which the sensitivity fields will be computed for a specified perturbation in the design variable. Figures 3.16, 3.17 and 3.18 show at $t = 50$ seconds the parameter sensitivity of the equivalent stress, state variable and temperature, respectively, using the CSM and FDM sensitivity computations.

The results from Examples 4-6 indicate that for both parameter and shape sensitivity problems, the solutions from the CSM sensitivity analysis approximate very well those obtained from the finite difference approach. The FDM computations for parameter and shape sensitivity analysis were performed using forward finite differencing with a 1% step size of the design parameters. Note that despite very large and non-homogeneous deformation, highly non-steady contact and friction conditions including new nodes abruptly coming in contact with the die (fold-over effect), the CSM and FDM results compare very well. This study therefore validates
Figure 3.15: The spatial variation of the equivalent stress, scalar state variable, plastic strain and temperature at \( t = 50 \) s (Example 6).

Figure 3.16: Spatial variation of the parameter sensitivity (FDM and CSM) of the equivalent stress at \( t = 50 \) s (Example 6).
Figure 3.17: Spatial variation of the parameter sensitivity (FDM and CSM) of the scalar state variable at $t = 50$ s (Example 6).

Figure 3.18: Spatial variation of the parameter sensitivity (FDM and CSM) of the workpiece temperature at $t = 50$ s (Example 6).
the thermo-mechanical sensitivity analysis implemented for four-noded quadrilateral
elements. More validation examples are available in [50, 51, 54, 59].

3.6 Optimization examples

3.6.1 Evaluation of gradients from the computed sensitivities

The gradients of various objective functions and constraints can be evaluated using
the sensitivity fields (directional derivatives) developed earlier. Assume that the
sensitivities of a continuum Lagrangian field \( \Omega(x, t; \beta) = \Omega(x, t; \beta_1, \beta_2, \ldots, \beta_n) \)
have been evaluated through the CSM problem where \( \beta \) is the vector denoting
the design parameters. The following can be written, through the definition of
sensitivities:

\[
\hat{\Omega}(x, t, \beta_1, \beta_2, \ldots, \beta_n, \Delta \beta_1, \Delta \beta_2, \ldots, \Delta \beta_n) \equiv \sum_{i=1}^{n} \frac{\partial \Omega}{\partial \beta_i} \Delta \beta_i \tag{3.70}
\]

Thus one can compute the gradient \( \nabla \Omega = (\frac{\partial \Omega}{\partial \beta_1}, \frac{\partial \Omega}{\partial \beta_2}, \ldots, \frac{\partial \Omega}{\partial \beta_n}) \) using the continuum
based sensitivity fields as:

\[
\frac{\partial \Omega}{\partial \beta_i} = \frac{\hat{\Omega}(x, t, \beta_1, \beta_2, \ldots, \beta_n, 0, \ldots, 0, \Delta \beta_i, 0, \ldots, 0)}{\Delta \beta_i} \tag{3.71}
\]

The evaluation of the gradient, therefore, requires \( n \) sensitivity problems where
the \( i^{th} \) sensitivity problem is driven by \( \Delta \beta_i \) with \( \Delta \beta_j = 0 \) for \( j \neq i \). Thus a total
of \( n + 1 \) problems are solved, one nonlinear direct problem and \( n \) linear sensitivity
problems. In comparison, the finite difference method (FDM) will need solutions
to \( n + 1 \) nonlinear direct problems to evaluate \( \nabla \Omega \). In addition to the anticipated
much higher accuracy of the CSM method versus the use of the FDM, significant
savings will thus result in terms of computational power.
3.6.2 Example 7: Preform design for closed-die forging - thermomechanical process with ductile damage

The objective of this problem is to design the volume and the free surface of a cylindrical preform of height 2.0 mm, that when forged with a closed die, fills the die cavity completely with minimum or no flash, after a specified stroke of 0.65 mm. The material of interest is 2024–T351 Al at an initial temperature of 300K. The material parameters correspond to those described in Appendix A.1. The friction coefficient between the die and workpiece is taken as 0.1. The desired final radius is 1.2 mm and the desired height at $r = 0$ is 0.7 mm. The particular die (i.e. the die profile $(r, z)$) for this problem is defined as:

![Guess preform](image1)

![Optimized preform solution](image2)

Figure 3.19: Comparing the final products obtained using the guess preform shape and the optimized preform shape (Example 7).
The finite dimensional optimization problem is posed as follows:

\[
\text{shape}(\eta) = \begin{cases} 
  r(\eta) = 1.6 \times (1 - \eta) \\
  0.9 & \eta \in [0, 0.25] \\
  4.1 - 25.6 \times \eta + 51.2 \times \eta^2 & \eta \in [0.25, 0.3125] \\
  10.35 - 105.6 \times \eta + \\
  371.2 \times \eta^2 - 409.6 \times \eta^3 & \eta \in [0.3125, 0.375] \\
  1.35 & \eta \in [0.375, 0.4375] \\
  -128.5 + 828.8 \times \eta - \\
  1753.6 \times \eta^2 + 1228.8 \times \eta^3 & \eta \in [0.4375, 0.5] \\
  9.1 - 28.8 \times \eta + 25.6 \times \eta^2 & \eta \in [0.5, 0.5625] \\
  1.0 & \eta \in [0.5625, 1]
\end{cases}
\]

where \( \eta \in [0, 1] \). Since the problem is complex in nature, it involves multiple remeshing operations. Remeshings are incorporated at different stages in the problem depending on the size of the elements in the mesh and the amount of distortion. The free surface \( R_\beta(\alpha) \) is represented with a degree 6 Bézier curve as in Section 3.5.1.

The finite dimensional optimization problem is posed as follows:

\[
\min_\beta \mathcal{F}(\beta) = \frac{1}{N} \sum_{i=1}^{N} (x_1^i(\beta) - x_1^{\text{desired}})^2 + (x_2^i(\beta) - x_2^{\text{desired}})^2 \quad (3.72)
\]

where \( \beta = \{\beta_1, \ldots, \beta_6\} \), \((x_1^{\text{desired}}, x_2^{\text{desired}})\) defines the desired boundary and \( N \) refers to the number of nodes on the free surface and regions in contact of the final product.

This objective function is non-dimensionalized using the volume of the die cavity, a constant parameter as the die is assumed rigid.

Figure 3.19 shows the quarter geometry of the initial guess preform (a right circular cylinder of radius 0.8mm and height 2mm) and the product obtained using this preform. In addition Figure 3.19 shows the optimal preform and the final product obtained using this optimal preform. Figure 3.20 compares the distribution of the shear modulus in the forged product, using the guess and optimized preforms.
The steepest descent optimization scheme is used and the variation of the objective function with the iteration index is shown in Figure 3.21. It can be observed from Figure 3.20: Comparison of the distributions of the shear modulus, in the finished product, through the two processes, using the guess preform shape and the optimized preform shape. (Example 7).

Figure 3.21: Variation of the nondimensionalized objective function with iteration index for a theromechanical closed die forming process (Example 7).

Figure 3.21 that the unfilled cavity is reduced by half after only 10 iterations. Similar optimization problems are also addressed in [59] and these examples highlight the capability of the design simulator to compute complex design solutions efficiently.
3.6.3 Example 8: Die design for extrusion to minimize Chevron cracking

Chevron defects, also known as central bursts, are gaps in the material flow that form a special category of ductile fracture. They lead to voids and cavities in the center of the workpiece making their detection extremely difficult. They can only be detected by full ultrasonic testing which increases the cost of the finished product. The objective of this problem is to design the extrusion die shape so as to minimize the void fraction at the center of the extruded product and thus avoid Chevron fracture. The extrusion process is designed for a fixed reduction in area of 10.7%. The initial radius of the workpiece is 0.508 mm and the initial length is 2.1 mm. The material is assumed to have an initial porosity of $f_o = 1\%$. The material was extruded with a nominal displacement rate of 0.01 s$^{-1}$ and a total of 120 time steps were performed. Frictionless conditions were assumed at the die-workpiece interface. The symmetry of the problem allowed modeling only half of the geometry. The die surface is represented by a degree nine ($n = 9$) Bézier curve as follows:

$$r(\alpha) = \sum_{i=1}^{n+1} C_i \phi_i(\alpha)$$

$$z = 0.2685(\alpha) \text{ in mm} \quad 0 \leq \alpha \leq 1 \quad (3.73)$$

where $C_i, i = [1\ldots(n+1)]$, are the algebraic control parameters, and $r$ and $z$ represent the radial and axial coordinates, respectively, of the die profile. The Bernstein functions $\phi_i(\alpha)$ are given as

$$\phi_1 = (1.0 - \alpha)^9$$

$$\phi_2 = 9.0 (1.0 - \alpha)^8 \alpha$$

$$\phi_3 = 36.0 (1.0 - \alpha)^7 \alpha^2$$

$$\phi_4 = 84.0 (1.0 - \alpha)^6 \alpha^3$$
\begin{align*}
\phi_5 &= 126.0 \ (1.0 - \alpha)^5 \alpha^4 \\
\phi_6 &= 126.0 \ (1.0 - \alpha)^4 \alpha^5 \\
\phi_7 &= 84.0 \ (1.0 - \alpha)^3 \alpha^6 \\
\phi_8 &= 36.0 \ (1.0 - \alpha)^2 \alpha^7 \\
\phi_9 &= 9.0 \ (1.0 - \alpha) \ \alpha^8 \\
\phi_{10} &= \alpha^9
\end{align*}

Constraints on the radius and slope (with respect to the z-axis) at the inlet and exit help to obtain and maintain the same required reduction for different die design parameters. These constraints are obtained as:

\begin{align*}
C_1 &= 0.508 \text{ mm} \\
C_{10} &= 0.48 \text{ mm} \\
C_2 &= C_1 \\
C_9 &= C_{10}
\end{align*}

With this selection of parameters, there are 6 die parameters that need to be optimized. The initial (reference) values are arbitrary and are selected as $C_3 = 0.508$; $C_4 = 0.49$; $C_5 = 0.49$; $C_6 = 0.485$; $C_7 = 0.485$; $C_8 = 0.485$ (all in mm). The flow rule and other material properties are discussed in Appendix A.4. The finite dimensional optimization problem is then posed as:

\[
\min_{\beta} \ F(\beta) = \frac{1}{N} \sum_{i=1}^{N} (f_i(\beta))^2
\]

where $\beta = \{\beta_1, \ldots, \beta_6\}$ are the unknown die parameters ($C_i$'s), $f^i$ is a sampling of void fractions along the extruded medium and $N$ refers to the total number of sampling nodal points of interest. A perturbation of $10^{-3}$ mm is used for evaluating the sensitivities with respect to the die shape. Figure 3.22 shows the geometry of the
Figure 3.22: Initial guess die shape and the final extruded product using this guess for an isothermal, frictionless extrusion process (Example 8).

Initial workpiece (a right circular cylinder of radius 0.508 mm and height of 2.1 mm) along with its discretization. Observe, in Figure 3.23, that the extruded product using the guess die shape has a void fraction $\geq 1\%$, the initial void fraction (e.g. look for the contour number 6). These are regions that could potentially develop Chevron cracks. Figure 3.23 also shows the distributions of the void fraction in the extruded product (obtained using the optimal die shape). The void fraction in the region of interest has decreased. In fact, the void fraction in this region (and elsewhere) is $< 1\%$. Also note that the void fraction in the periphery of the workpiece has increased compared to that of the initial product, even though it is much lower than the initial void fraction. The variation of the die shape for different optimization iterations is shown in Figure 3.24.
Figure 3.23: Initial and optimal distribution of volume void fraction in the final product for an extrusion process (Example 8).

Figure 3.24: Variation of the die shapes for different optimization iterations (Example 8).
3.6.4 Example 9: Multi-stage design: Die design in open-die hot forging to minimize barrelling

In industrial forming applications, objectives based on complex material and property descriptions can seldom be achieved by a single forming operation. As a result, intermediate deformation or preforming steps are used to efficiently transform the initial geometry into a final shape with desired material properties. One such case is addressed through this example. Commonly, a forming process sequence can be viewed at two broad levels of design: (1) To identify specifically the number, type and order of thermo-mechanical operations and (2) A priori selection of a process sequence and then using an optimization framework for the specific identification and selection of design variables in each of the forming operations. The problem of interest in this example falls under the second category.

An initial workpiece in the form of a right circular cylinder of radius $r = 1.0$ mm and height 2.0 mm is considered. The objective in this example is to design the die shape in the preforming stage (first stage of a 2-stage process), so that the product after the finishing stage (second stage) is also right circular cylinder with a radius $r_o = 1.414$ mm and height 1.0 mm. The height reduction at $r = 0$, in the first stage is to be 0.6 mm and in the second stage is the remaining 0.4 mm. The friction coefficient for both stages is taken as 0.2, the initial workpiece temperature is set at 673 K and the heat transfer coefficients are taken as $h_0 = h_c = 6.7 \text{ W/m}^2\text{K}$. The die contact surface is represented using a degree 6 Bézier curve with 5 independent variables, similar to the parametrization in Section 3.6.3:

$$r(\alpha) = 1.5\alpha, \quad z_\beta(\alpha) = \sum_{i=1}^{7} \beta_i \phi_i(\alpha)$$

(3.80)

The die height at $r = 0$ was specified and because of symmetry the die shape is
assumed to have a zero slope at \( r = 0 \). The following basis functions

\[
\phi_1 = (1 - \alpha)^6, \quad \phi_2 = 6(1 - \alpha)^5\alpha, \quad \phi_3 = 15(1 - \alpha)^4\alpha^2, \quad \phi_4 = 20(1 - \alpha)^3\alpha^3, \\
\phi_5 = 15(1 - \alpha)^2\alpha^4, \quad \phi_6 = 6(1 - \alpha)\alpha^5, \quad \phi_7 = \alpha^7
\]  

(3.81)

are assumed. It is further chosen that \( \beta_6 \) and \( \beta_7 = 1.3 \) mm, in order to fix the height and slope at \( r = 0 \).

The finite dimensional optimization problem is then posed as:

\[
\min_{\beta} f(\beta) = \frac{1}{M} \sum_{i=1}^{M} (x_i(\beta) - r_o)^2
\]  

(3.82)

where \( \beta = \{\beta_1, \ldots, \beta_5\} \) and \( M \) refers to the number of nodes on the free surface of the final product (which can vary in between optimization iterations). A straight (flat) die is chosen as the initial (guess) preforming die. The steepest descent method with optimal step size selection is used to perform the optimization. The variation of the objective function with the iteration index is shown in Figure 3.25. Results show that convergence is achieved in about 12 iterations. Figure 3.26 shows the initial, intermediate and optimal solution of the preforming die shape as well as the shapes of the products at various stages of the processing operation.
Figure 3.25: Variation of the objective function which quantifies the amount of barreling in the final product versus the optimization iteration index (Example 9).

Stage 1 - preforming

Stage 2 - finishing

Figure 3.26: Optimal solution for the thermo-mechanical preform forging design problem minimizing barreling (Example 9).
Chapter 4

A multi-length scale approach towards modeling thermo-mechanical processes

Material properties and processing techniques are severely affected by the underlying microstructural features in the material. These microstructural features include texture, grain sizes and shapes, grain boundary motion and secondary phase particles, etc., and their adequate representation is necessary for an accurate prediction of material response. Polycrystal models have primarily characterized the polycrystal through a discrete aggregate of crystals, as in [8]-[15]. This approach works on the idea of combining discrete, preselected, single crystal responses with a suitable macro-micro linking hypothesis. Such discrete aggregate models, though simple, do not characterize texture effectively. There also exists no means by which one can compare and quantify differences between textures associated with distinct discrete aggregates. An alternate approach is a continuum representation of crystals based on quantifying texture through an Orientation Distribution Function (ODF) which
expresses the distribution of crystal orientations over the orientation space [57]. In these methods, the evolution of a polycrystal generally requires that an ODF conservation equation be solved numerically. The common implementation techniques, for continuum representations, are based on the series representation of the ODF through schemes like spherical harmonics, infinite polynomial series or tensorial Fourier series. These schemes are not only complex but also lack the capability to adequately represent sharp textures. In order to overcome the above mentioned difficulties, the approach developed in [16, 19] is used, where the ODF was defined through finite element piecewise polynomial functions over an explicit discretization of the orientation space. The advantages of such an approach are substantial and are discussed in detail in [19].

Over the last four decades, researchers have also been interested to study the plastic anisotropy developed during deformation and to formulate models that predict experimentally observed behavior ([24]-[33]). Most models for crystalline materials are restrictive in the sense of a limited operating region of processing conditions. However modern applications lie in a very broad operating regime - in terms of both strain rates and operating temperatures. Critical investigations to develop accurate descriptions of material behavior (incorporating thermal response) include [23, 28]. In order to model thermal effects, it is necessary to understand the thermal activation of dislocations. The activation rate of dislocation events depends on the frequency of attempts on overcoming an obstacle. This frequency is modeled, as in [28], by a Boltzmann distribution. The activation energy further depends on the temperature and is the difference between the activation enthalpy and the free enthalpy (Gibbs free energy) of an obstacle. Much of the background information on the effects of varying temperatures on texture is discussed extensively in [23]. More
recently, Anand and Colleagues [8, 12] have developed improved kinetic equations for the shearing rates on slip systems and have compared the response for b.c.c Tantalum and f.c.c Aluminium with experimentally available results. This theory has been motivated by the thermal activation theory for plastic flow and is used as the basis in this study.

As part of this chapter, a multi-length scale framework is developed to model material behavior. In Section 4.1, the continuum description of polycrystals, to be used in the elasto-viscoplastic framework, is briefly introduced. In Section 4.2, crystal-mechanics and the constitutive model for polycrystalline materials is developed followed by a solution methodology to compute the re-orientation in Section 4.3. In particular, two approaches have been developed - a Eulerian approach for modeling texture evolution based on an earlier work by Kumar and Dawson [20] and a Lagrangian approach for modeling thermo-elasto viscoplastic responses [60]. Section 4.4 provides details on the solution of the kinematic problem (in the context of a multi-length scale analysis) including a calculation of the material moduli. In Section 4.5, the development of a reduced-order model, in an Eulerian framework, is addressed. Section 4.6 considers a set of examples to demonstrate the accuracy, performance and applicability of the proposed algorithms.

4.1 Overview of microstructure in polycrystalline materials

For accurately modeling the response of polycrystals undergoing deformation, one needs to be able to accurately represent polycrystals. One of the most common techniques for representing polycrystals is based on the use of a collection of discrete
grains/orientations. Such an approach needs the choice of the grain orientations to accurately represent the texture in the material. An alternative approach has been to use statistical methods like Monte-Carlo and Cellular Automaton to simulate the polycrystal. These approaches, though uncommon for modeling texture evolution during plastic deformation, are very common when simulating recrystallization and recovery in polycrystalline materials [61]-[67]. The emphasis in this thesis is on a continuum representation of polycrystals, based on the pioneering work of Kumar and Dawson in [16]-[20].

Remark 2: Even though, the goal of this thesis is not to reinvent or reproduce the original work of Kumar and Dawson [16, 19, 20], it is strongly felt that a brief overview of the continuum methodology developed by these researchers will help develop a clearer understanding of the contributions of this thesis. Furthermore, to maintain continuity of the work pioneered by Kumar and Dawson, the notations developed in [19] are utilized in future discussions.

Consider a macroscopic material point and let it be associated with the underlying microstructure \( \mathcal{M} \). Assume that the response of any crystal of the polycrystal is determined only by its orientation \( \mathbf{R} \), which is the rotation relating the crystal lattice frame, \( \hat{\mathbf{e}}_i \), to a sample reference frame \( \mathbf{e}_i \) as \( \mathbf{e}_i = \mathbf{R} \hat{\mathbf{e}}_i \). The orientation \( \mathbf{R} \in \mathcal{O}^+ \) is not unique because of crystal symmetries. This non-uniqueness has traditionally been resolved by restricting the choice of orientation to a fundamental region of \( \mathcal{O}^+ \). Thus for a particular choice of the fundamental region \( \mathcal{R} \), the orientation of the crystal is uniquely represented by \( \mathbf{r} \in \mathcal{R} \) where

\[
\mathbf{R} = \mathcal{Q}(\mathbf{r}) \tag{4.1}
\]

and \( \mathcal{Q} \) maps the orientation space to the set of all proper orthogonal tensors. The notion of crystals being interchangeable with unique parametrized orientations
Figure 4.1: A Lagrangian framework describing the association of a polycrystal, at a material point $X$, with unique parameters $s$ and $r$, drawn from the fundamental region. Also shown is the re-orientation vector $\hat{r}(s, t)$. 
is developed in [19]. This is then used to define texture as a map of crystals to orientations within the fundamental region. A microstructure, $M$, is then associated with a collection of such mappings, $\Phi$, so that each map, $\chi \in \Phi$, is a one-to-one mapping of the microstructure $M$ onto the fundamental region $R$. Further, the orientation of a crystal, $r$, is developed as

$$ r = \chi(p) \quad (4.2) $$

where $p$ represents the crystals associated with the microstructure $M$. A graphical representation of this framework is shown in Figure 4.1. Through such a description, microstructure is treated as a continuum of crystals, that under the map $\chi$ occupies a fundamental region of the orientation space. The ODF, represented as $A(r)$, describes the crystal density over the fundamental region. The ODF is defined so that the crystal volume fraction for any part $M^* \subseteq M$,

$$ v_f(M^*) = \int_{\chi(M^*)} A(r)dv \quad (4.3) $$

is independent of the map $\chi$. $dv$ is the volume element on the reference fundamental region. $M$ can also be associated with a family of maps $\chi_t$ which take a crystal to the fundamental region $R_t$. Such a description helps in modeling time dependent texturing. Let $\chi$ be the reference map and correspondingly $R$ is the reference fundamental region. The family of maps $\chi_t$ along with the reference map $\chi$ determine a family of mappings $\hat{r}(\bullet, t) : R \rightarrow R_t$ referred to as the re-orientation, and given by (see Figure 4.1)

$$ \hat{r}(s, t) = \chi_t(\chi^{-1}(s)) \quad (4.4) $$

The re-orientation vector, $\hat{r}$, is associated with the one-parameter family of ODF’s,

$$ A(r, t) = A_{\chi_t}(r) = A(\hat{r}(s, t), t) = \hat{A}(s, t). $$

The representation of the ODF given by $A(r, t)$ is Eulerian and $\hat{A}(s, t)$ is Lagrangian.
Consider the integral conservation equation, Equation (4.3). Applying this conservation equation to arbitrary parts $M^* \subseteq M$ under maps $\chi$ and $\chi_t$, followed by a transformation of variables to the reference fundamental region, results in the following

$$\int_{\chi(M^*)} (\dot{A}(s, t) J(s, t) - \dot{A}(s, 0)) \, dv = 0$$

(4.5)

where $J(s, t) = \det(\nabla \hat{r}(s, t))$ is the Jacobian determinant of the re-orientation of the crystals and $\dot{A}(s, 0) = A_0(s)$ is the ODF associated with the reference map and can be thought of as the initial texturing of the material. The Lagrangian version of the conservation equation is then defined as [19]

$$\dot{A}(s, t) J(s, t) = \dot{A}(s, 0) = A_0(s)$$

(4.6)

The conventional Eulerian rate form of the conservation equation is obtained by considering the rate of Equation (4.6) as

$$\frac{\partial A(r, t)}{\partial t} + \nabla A(r, t) \cdot v(r, t) + A(r, t) \nabla \cdot v(r, t) = 0$$

(4.7)

where $v(r, t)$ is the Eulerian re-orientation velocity. Such an Eulerian representation of the ODF is useful in cases where elastic effects are negligible. Examples of works utilizing such a framework include [19, 20, 58, 59]. In a Lagrangian framework, the re-orientation, $\hat{r}$, has to be evaluated from the re-orientation velocity $\hat{v}(s, t) = v(\hat{r}(s, t), t) = v(r, t)$ through the following relation

$$\frac{\partial \hat{r}}{\partial t}(s, t) = \hat{v}(s, t)$$

(4.8)

Texture evolution is thus modeled by an ODF at each of the material points of the macro-continuum (see Figure 4.1).

For completeness, the neo-Eulerian parametrization of $R$ is also briefly described. The parametrization of $R$ is derived from the natural invariants of $R$: the axis of
rotation $\mathbf{n}$ and the angle of rotation $\xi$. The angle-axis parametrization, $r$, is obtained by scaling the axis $\mathbf{n}$ by a function of the angle $\xi$ as $r = \mathbf{n} f(\xi)$. In the particular case of Rodrigues’ parametrization, the function is defined as $f(\xi) = \tan \left( \frac{\xi}{2} \right)$. In this case, the orientation $\mathbf{R}$ is related to the parametrization $r$ as

$$
\mathbf{R} = Q(r) = \frac{1}{(1 + r \cdot r)} \left\{ I(1 - r \cdot r) + 2(r \otimes r + I \times r) \right\}
$$

(4.9)

where $I$ is the second order identity tensor and $\otimes$ denotes the tensor product of the two quantities. The ODF, in the present work, is approximated with finite element polynomial functions defined over an explicit discretization of the orientation space based on Rodrigues’ parametrizations. The Rodrigues’ parametrization was chosen over pole figures or Euler angle spaces because of its several advantages, discussed in detail in [19]. In fact, if the initial texturing is known, and the re-orientation of the crystal orientations is computed during deformation, then the current mapping or the current Lagrangian ODF can be evaluated using Equation (4.6). The polycrystal average of an orientation dependent property, $\Upsilon(r, t)$, is determined as:

$$
\langle \Upsilon \rangle = \int_{\mathcal{R}_t} \Upsilon(r, t) \, A(r, t) \, dv_t
$$

$$
= \int_{\mathcal{R}} \Upsilon(\hat{r}(s, t), t) \, A_0(s) \, dv
$$

(4.10)

where $dv_t$ is defined as the volume element on the current fundamental region. From Equation (4.10), one can conclude that if the re-orientation and the initial texture are known, then the average property for the polycrystal can be evaluated. Thus, there is no reason to compute the current ODF, $\hat{A}(s, t)$ or $A(r, t)$. Hence these methods have no computational disadvantages over the discrete framework.
4.2 The constitutive problem

During a deformation process, crystallographic slip and re-orientation of crystals (lattice rotation) can be assumed to be the primary mechanisms of plastic deformation. The slip and re-orientation occur in an ordered manner such that a preferential orientation or texture develops. Most of the constitutive models, currently in use for polycrystalline plasticity, are restricted to a small range of temperatures and strain rates. Frost and Ashby [23] introduced deformation maps for polycrystalline materials along with a summary of thermal activation theories in literature. There have been several significant contributions by other authors as well [8, 11, 12, 28, 32, 68]. In order to model thermal effects, it is necessary to understand the thermal activation of dislocations. The activation rates of dislocation events is given by a Boltzmann distribution [28]. The activation energy further depends on the temperature. At absolute zero, the slip system resistance \( s^\alpha(0) \), of slip system \( \alpha \) (referred to as the mechanical threshold by Kocks [28]) has to be completely overcome by the resolved shear stress, \( \tau^\alpha \). At temperatures greater than absolute zero, short-range obstacles can be overcome at a lower stress level with the help of the additional thermal energy. Obstacles can therefore be classified as thermal and athermal [23]. The thermal barriers, in metals, include the Peierls stress, forest dislocations and weak precipitates whereas large and strong precipitates are examples of the athermal barriers. In metals without large precipitates, since it is known that the thermal energy is sufficient to overcome short range barriers, the constitutive formulations are expressed in terms of the thermal part of the resolved shear stress and the thermal part of the shearing resistance.

The constitutive framework is briefly summarized next. Consider a point on the reference fundamental region and this corresponds to a particular crystal orientation.
Figure 4.2: Schematic of the various material configurations, for a single crystal, used in the integration of the constitutive model. \( \mathbf{m}^\alpha \) denotes the slip direction and \( \mathbf{n}^\alpha \) denotes the slip normal. These together define the slip systems and are assumed to be known on the reference (initial) configuration. The Schmid tensor is evaluated as \( S_0^\alpha = \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha \). \( \hat{\mathbf{m}}^\alpha \) and \( \bar{\mathbf{m}}^\alpha \) are the slip directions in the deformed configurations (different from \( \mathbf{m}^\alpha \) because of crystal re-orientation). Similarly, \( \hat{\mathbf{n}}^\alpha \) and \( \bar{\mathbf{n}}^\alpha \) are the slip normals in the deformed configurations \( \mathcal{B}_n \) and \( \mathcal{B}_{n+1} \), respectively. \( F_r \) is the relative deformation gradient from \( \mathcal{B}_n \) to \( \mathcal{B}_{n+1} \).
In an appropriate kinematic framework, such as the one introduced in [44] for large deformation inelastic analysis, the total deformation gradient is decomposed into plastic and elastic parts as follows (Figure 4.2):

$$F = F^e F^p$$  \hspace{1cm} (4.11)

where $F^e$ is the elastic deformation gradient and $F^p$, the plastic deformation gradient, with $\det F^p = 1$. In this analysis, the Taylor hypothesis is utilized as the macro-micro linking assumption. As a result of this assumption, the crystal deformation gradient (in the sample reference frame) is taken to be the same as the macroscopic deformation gradient. This linking assumption and the particular choice of decomposition of the deformation gradient results in:

$$F^e = F (F^p)^{-1}$$  \hspace{1cm} (4.12)

It is further assumed that deformation takes place through dislocation glide and the evolution of the plastic flow is given by

$$\dot{F}^p (F^p)^{-1} = \bar{L}^p = \sum_\alpha \dot{\gamma}^\alpha S^\alpha_0$$  \hspace{1cm} (4.13)

where $S^\alpha_0 = m^\alpha \otimes n^\alpha$ is the Schmid tensor, $\dot{\gamma}^\alpha$ is the plastic shearing rate on the slip system $\alpha$ and $m^\alpha$ and $n^\alpha$ are the slip directions and the slip plane normals respectively. Figure 4.2 clearly describes the constitutive problem along with the slip systems in different configurations. An Euler-backward time integration procedure leads to the following approximation:

$$F^p = \exp(\Delta t \sum_\alpha \dot{\gamma}^\alpha S^\alpha_0) F^p_n \approx (I + \Delta t \sum_\alpha \dot{\gamma}^\alpha S^\alpha_0) F^p_n$$  \hspace{1cm} (4.14)

for small $\Delta t$. Substituting Equation (4.14) into Equation (4.12) results in the following:

$$F^e = F^e_{trial}(I - \Delta t \sum_\alpha \dot{\gamma}^\alpha S^\alpha_0)$$  \hspace{1cm} (4.15)
where $F^e_{\text{trial}}$ is the trial elastic deformation gradient and is given as $F^e_{n+1}(F^p_n)^{-1}$.

In the constitutive equations to be defined below, the Green elastic strain measure defined on the relaxed configuration (plastically deformed, unstressed configuration) $\bar{B}$ is utilized. It is computed using Equation (4.15) as

$$
\bar{E}^e = \frac{1}{2} \left( \bar{F}^e T \bar{F}^e - I \right) \tag{4.16}
$$

$$
\bar{E}^e = \bar{E}^e_{\text{trial}} - \frac{\Delta t}{2} \sum_\alpha \dot{\gamma}^\alpha \left( (S^\alpha_0)^T \bar{F}^e_{\text{trial}} T F^e_{\text{trial}} + (F^e_{\text{trial}})^T F^e_{\text{trial}} S^\alpha_0 \right) \tag{4.17}
$$

where $\bar{F}^e_{\text{trial}} = \frac{1}{2} \left( (F^e_{\text{trial}})^T F^e_{\text{trial}} - I \right)$.

The conjugate stress measure is then defined as

$$
\bar{T} = \text{det} F^e (F^e)^{-1} T (F^e)^{-T} \tag{4.18}
$$

where $T$ is the Cauchy stress for the crystal in the sample reference frame. All vector and tensorial quantities are expressed in the sample reference frame. Furthermore, crystal specific properties like the stiffness and compliance have to be transformed to this sample reference frame using the crystal orientation $r$. The constitutive relation, for stress, for small temperature changes about the initial temperature, $\theta_0$, is given by

$$
\bar{T} = \mathbf{L}^e \left[ \bar{E}^e - A(\theta - \theta_0) \right] \tag{4.19}
$$

where $\mathbf{L}^e$ is the fourth-order anisotropic elasticity tensor expressed in terms of the crystal stiffness parameters and the orientation $r$, and $A$ is the second-order anisotropic thermal expansion tensor. Using Equation (4.17) in Equation (4.19) results in the following

$$
\bar{T} = \bar{T}_{\text{trial}} - \frac{\Delta t}{2} \sum_\beta \dot{\gamma}^\beta \mathbf{L}^e \left[ (S^\beta_0)^T \bar{F}^e_{\text{trial}} T F^e_{\text{trial}} + (F^e_{\text{trial}})^T F^e_{\text{trial}} S^\beta_0 \right] - (\theta - \theta_0) \mathbf{L}^e [A] \tag{4.20}
$$

where $\bar{T}_{\text{trial}} = \mathbf{L}^e \left[ \bar{E}^e_{\text{trial}} \right]$. 
Further, if \( s^\alpha(\theta) \) is the slip system resistance at temperature \( \theta \) K, then \( s^\alpha(\theta) < s^\alpha(0) \). It is also known that part of the resolved shear stress has to overcome the athermal barriers. The thermal barriers can be overcome by a combination of thermal energy and the resolved shear stress. Thus the thermal and athermal components of the slip system resistance and the resolved shear stress are defined as

\[
\begin{align*}
    s^\alpha &= s^\alpha_{at} + s^\alpha_t \quad (4.21) \\
    \tau^\alpha_t &= |\tau^\alpha| - s^\alpha_{at} \quad (4.22)
\end{align*}
\]

where the subscripts \( t \) and \( at \) denote the thermal and athermal parts, respectively and \( \tau^\alpha \), the resolved shear stress for the \( \alpha^{th} \) slip system, is computed as \( \bar{T} \cdot S_0^\alpha \).

The shearing rate can then be expressed as (refer to Chapter 2 in [23])

\[
\dot{\gamma}^\alpha = \begin{cases} 
0 & \tau^\alpha_t \leq 0 \\
\dot{\gamma}^0 \exp \left\{ -\frac{\Delta G^\alpha(\tau^\alpha_t, s^\alpha_t)}{k_B\theta} \right\} \text{sign}(\tau^\alpha), & 0 < \tau^\alpha_t < s^\alpha_t
\end{cases} \quad (4.23)
\]

where, the activation enthalpy is given by

\[
\Delta G^\alpha(\tau^\alpha_t, s^\alpha_t) = \Delta F^\alpha \left[ 1 - \left( \frac{\tau^\alpha_t}{s^\alpha_t} \right)^p \right]^q \quad (4.24)
\]

In the equation above, \( \Delta F^\alpha \) is the activation energy at 0K, \( p \) and \( q \) are material parameters (generally, \( 0 < p < 1 \) and \( 1 < q < 2 \)) and \( k_B \) is the Boltzmann constant. Furthermore, the slip system resistance parameters \( s^\alpha_{at} \) and \( s^\alpha_t \) evolve with deformation as

\[
\dot{s}^\alpha = \sum_\beta h^{\alpha\beta} |\dot{\gamma}^\beta| \quad (4.25)
\]

and \( h^{\alpha\beta} \) is defined as

\[
\begin{align*}
    h^{\alpha\beta} &= q^{\alpha\beta} h^\beta \quad (\text{no sum on } \beta) \\
    h^\beta &= h_0^\beta \left| 1 - \frac{s^\beta}{s^\beta s}_r \right| \text{sign} \left\{ 1 - \frac{s^\beta}{s^\beta s} \right\} \quad (4.27)
\end{align*}
\]
In Equation (4.26), $q^{\alpha\beta}$ represents the latent-hardening parameter with the following property

$$q^{\alpha\beta} = \begin{cases} 1 & \text{if } \alpha = \beta \\ q_h = 1.4 & \text{if } \alpha \neq \beta \end{cases}$$  \hspace{1cm} (4.28)

Further, $s_\beta^\beta$ represents the saturation value of $s^\beta$, $h_0^\beta$ and $r_1$ are material response parameters. It is normally assumed, for b.c.c materials, that the thermal part of the slip system resistance, $s^\alpha_t$, is a constant and thus the above equations lead to the rate equations for the athermal part of the slip system resistance [8]. For f.c.c materials, both the thermal and athermal parts of the slip system resistance evolve with strain and contribute to the macroscopic strain hardening. The experimental results in [69] have shown that the ratio $s^\alpha_t / s^\alpha_{at}$ is independent of the strain over a range of strains. This ratio is denoted by the parameter $\eta$ where

$$\eta = \frac{s^\alpha_t}{s^\alpha_{at}}$$  \hspace{1cm} (4.29)

and $0.5 \leq \eta \leq 1$. Furthermore, for f.c.c materials, $s_\beta^\beta$, the saturation state of $s^\beta$, can be expressed as a function of the strain rate and temperature, but will be considered as a constant in this work.

An Euler-backward time integration of Equation (4.25) along with Equations (4.26) and (4.27) result in the following

$$s^\alpha_{n+1} = s^\alpha_n + \Delta t \sum_\beta q^{\alpha\beta} g^\beta (r_{\beta n+1}^\beta, s^\beta_{n+1}, \theta)$$  \hspace{1cm} (4.30)

where $g^\beta = h^\beta |\dot{\gamma}^\beta|$. This state equation can be used for both b.c.c and f.c.c materials. With b.c.c materials, $s^\alpha_t$ is a constant. Therefore the athermal component is expressed as

$$s^\alpha_{at} = s^\alpha_{n+1} - s^\alpha_t$$  \hspace{1cm} (4.31)
Similarly, for f.c.c materials, the ratio \( \eta = \frac{s_{at}^{\alpha}}{s_{st}^{\alpha}} \), which is a constant, is utilized to evaluate the thermal and athermal parts of slip system hardness as

\[
\begin{align*}
    s_{at}^{\alpha} &= s_{n+1}^{\alpha} \frac{1}{1 + \eta} \\
    s_{t}^{\alpha} &= s_{n+1}^{\alpha} \frac{\eta}{1 + \eta}
\end{align*}
\]  

(4.32)

(4.33)

In addition, the plastic work contributes to the internal heating of the material.

This plastic work rate per unit volume is computed as

\[
\dot{\mu}_{p} = \int R \sum_{\alpha} (\tau_{\alpha} \dot{\gamma}_{\alpha}) A_{0} dv
\]  

(4.34)

The procedure for the evaluation of the resolved shear stress \( \tau_{\alpha} \) and the slip system resistance \( s_{\alpha} \) is described in Box 3. Finally, the re-orientation velocity can be evaluated [16] as:

\[
v = \frac{\partial \mathbf{r}}{\partial t} = \frac{1}{2} (\mathbf{\omega} + (\mathbf{\omega} \cdot \mathbf{r}) \mathbf{r} + \mathbf{\omega} \times \mathbf{r})
\]  

(4.35)

where \( \mathbf{r} \) is the orientation (Rodrigues’ parametrization) and \( \mathbf{\omega} \) represents the spin vector defined as \( \mathbf{\omega} = \text{vect} \left( \dot{\mathbf{R}}^{e} \mathbf{R}^{eT} \right) = \text{vect} (\Omega) \) where \( \dot{\mathbf{R}}^{e} \) is evaluated through the polar decomposition of the elastic deformation gradient \( \mathbf{F}^{e} \) as \( \mathbf{F}^{e} = \mathbf{R}^{e} \mathbf{U}^{e} \).

Considering the Euler-backward time integration of \( \dot{\mathbf{R}}^{e} \mathbf{R}^{eT} = \Omega \), where \( \Omega \) is the spin tensor, leads to the following:

\[
\mathbf{R}^{e}_{n+1} = \exp(\Delta t \Omega_{n+1}) \mathbf{R}^{e}_{n}
\]  

(4.36)

and

\[
\Omega_{n+1} = \frac{1}{\Delta t} \ln \left\{ \frac{\mathbf{R}^{e}_{n+1} \mathbf{R}^{eT}_{n}}{\mathbf{R}^{e}_{n} \mathbf{R}^{eT}_{n+1}} \right\}
\]  

(4.37)

Once the constitutive problem is solved (i.e. Box (1) is solved), \( \mathbf{F}^{e}_{n+1} \) can be evaluated from Equation (4.15). From the elastic deformation gradients, \( \mathbf{R}^{e}_{n+1} \) and \( \mathbf{R}^{e}_{n} \) are evaluated and one can evaluate the spin tensor \( \Omega_{n+1} \) using Equation (4.37) and
then the re-orientation velocity from Equation (4.35). Furthermore, post-processing involves computing the average Cauchy stress from

\[
\langle \mathbf{T} \rangle = \int_{\mathcal{R}} \mathbf{T}(\mathbf{\dot{r}}(\mathbf{s}, t), t) \mathcal{A}_0(\mathbf{s}) \, dv
\]  

(4.38)

- Simultaneously solve the system of equations (Equations (4.39) & (4.40)) for \( \tau \) and \( s \). The first system of equations can be derived from Equation (4.20) by taking the dot product with \( \mathbf{S}_0^\alpha \). The system of Equations (4.40) is simply Equations (4.30) introduced earlier by integrating the slip system hardening equations.

\[
\mathcal{M}_1^\alpha \equiv \tau_{n+1}^\alpha - \tau_{\text{trial}}^\alpha + \frac{\Delta t}{2} \sum_{\beta} \{ \dot{\gamma}_{n+1}^\beta \mathcal{L}^e \left[ \mathbf{B}^\beta \right] \cdot \mathbf{S}_0^\alpha \} \\
+ (\theta - \theta_0) \mathcal{L}^e [\mathbf{A}] \cdot \mathbf{S}_0^\alpha = 0 \quad (4.39)
\]

\[
\mathcal{M}_2^\alpha \equiv s_{n+1}^\alpha - s_n^\alpha - \Delta t \sum_{\beta} q^{\alpha\beta} g_{n+1}^\beta = 0 \quad (4.40)
\]

where \( \mathbf{A} \) is the anisotropic thermal expansion tensor, \( \tau_{\text{trial}}^\alpha = \mathbf{L}^e (\mathbf{E}_\text{trial}^e) \cdot \mathbf{S}_0^\alpha \) is the trial resolved shear stress and \( \mathbf{B}^\beta = \left\{ (\mathbf{S}_0^\beta)^T (\mathbf{F}_\text{trial}^e)^T \mathbf{F}_\text{trial}^e + (\mathbf{F}_\text{trial}^e)^T \mathbf{F}_\text{trial}^e \mathbf{S}_0^\beta \right\} \). Further, \( \dot{\gamma}_{n+1}^\beta \) and \( g_{n+1}^\beta \) are both functions of \( (\tau_{n+1}, s_{n+1}^\beta \) and \( \theta \) making Equations (4.39) & (4.40) a coupled nonlinear system of equations.

- Equations (4.39) & (4.40) are solved using a Newton-Raphson approach with line search. The tolerances for convergence were taken as \( 10^{-5} s_0^\alpha \) and initially all slip systems were assumed to have the same slip system resistance, \( s_0^\alpha \).

Box 3: Coupled system for the computation of the resolved shear stress and slip system hardenness.
4.3 Calculating the re-orientation given the re-orientation velocity

Consider the re-orientation velocity defined in Equation (4.35). It can be rewritten as:

\[
\frac{\partial r}{\partial t} - M_1 r = \frac{1}{2} \omega \tag{4.41}
\]

where \( M_1 = \frac{1}{2} \{ \Omega + (\omega \cdot r) I \} \) and \( \omega = \text{vect}(\Omega) \). Assuming small time steps and applying an Euler-backward time integration scheme, leads to the following linear system:

\[
r_{n+1} = \left\{ I + \frac{\Delta t}{2} (\Omega + (\omega \cdot r_{n+1} I)) \right\} r_n + \frac{\Delta t}{2} \omega, \tag{4.42}
\]

which can be solved for \( r_{n+1} \) to compute the current fundamental region. Note that the spin vector, \( \omega \), is computed at the quadrature points. Thus to use the equation above to obtain the nodal reorientation velocities, one needs to project \( \omega \) onto the nodes in the finite element discretization of the reference fundamental region. The actual projection error transferred to the re-orientation is reduced by a factor corresponding to the small time step used in the algorithm (as seen from Equation (4.42)). Thus if the initial orientation (fundamental region) is accurate, it is reasonable to expect accurate description of the fundamental region at different times.

An alternate procedure for computing the deformed fundamental region is to directly use \( R^e_{n+1} \), obtained from the polar decomposition of the elastic deformation gradient \( F^e_{n+1} \) to compute \( r_{n+1} \). This can be achieved through an inverse map derived from Equation (4.9). It has to be noted that the neo-Eulerian parametrization of an orientation, \( R \), is unique if a particular fundamental region is chosen (or known). In the present case, however, the current fundamental region, which is
defined by \( r_{n+1} \), is unknown. Thus there are many parametrizations that reproduce the orientation \( R \). Each such parametrization results in one choice of the current fundamental region. Furthermore, if such an \( r_{n+1} \) is found, it would correspond to the quadrature points in the finite element discretization of the fundamental region and a smoothing operation, with an associated projection error, needs to be performed. This alternative method for computing \( r_{n+1} \) was thus not further investigated in this work. Finally, it is important to mention that due to the Lagrangian nature of the analysis, one needs to ensure that at large strains the finite element discretization of the current fundamental region is acceptable and this generally requires remeshing and data transfer operations.

### 4.4 Solution of the kinematic problem

A total Lagrangian framework is adopted for the kinematic problem, in contrast to the kinematic problem discussed in Chapter 2. The equilibrium equation is expressed on the reference configuration, based on the polycrystal plasticity approach highlighted earlier, as:

\[
\nabla_0 \cdot \langle P \rangle + f = 0
\]

(4.43)

where \( \nabla_0 \cdot \) represents the divergence in the reference/initial configuration (total Lagrangian approach). The polycrystal average Piola-Kirchhoff-I stress, \( \langle P \rangle \) is expressed as

\[
\langle P \rangle = \langle \det F \ T \ F^{-T} \rangle = \det F \langle T \rangle \ F^{-T}
\]

(4.44)

using the Taylor hypothesis for the macro-micro linking assumption. The incremental quasi-static problem is to determine the displacement field or the incremental
displacement field that satisfies Equation (4.43). The weak form of this equation, for any kinematically admissible test function \( \tilde{\mathbf{u}} \), is written as

\[
\mathcal{G}(\mathbf{u}_{n+1}, \tilde{\mathbf{u}}) \equiv \int_{B_0} \langle P \rangle \cdot \nabla_0 \tilde{\mathbf{u}} dV - \int_{\partial B_0} \lambda_\bullet \tilde{\mathbf{u}} dA - \int_{B_0} \mathbf{f}_\bullet \tilde{\mathbf{u}} dV = 0 \tag{4.45}
\]

where the applied surface traction \( \lambda \) and body forces \( \mathbf{f} \) are given. It is further assumed that the contact problem is independent of the nature of the underlying microstructure, and that texture plays a role in this equation only through the stress response. To solve this non-linear equation, a Newton-Raphson iterative scheme along with a line search procedure, detailed in Chapter 2, is employed. The linearization process of the micro-averaged PK-I stress is given by [60]:

\[
\delta \langle P \rangle = \det \mathbf{F} \left( \text{tr}(\delta \mathbf{F} \mathbf{F}^{-1}) \langle \mathbf{T} \rangle - \langle \mathbf{T} \rangle \left( \delta \mathbf{F} \mathbf{F}^{-1} \right)^T + \langle \mathbf{C} \left[ \delta \mathbf{E}^e_{\text{trial}} \right] \rangle \right) \mathbf{F}^{-T} \tag{4.46}
\]

where \( \mathbf{C} \) denotes the consistent tangent moduli for a single crystal orientation, defined as

\[
\mathbf{C} = \frac{\partial \mathbf{T}}{\partial \mathbf{E}^e_{\text{trial}}} \tag{4.47}
\]

Considering the linearization of Equation (4.20), one obtains:

\[
\delta \mathbf{T} = \mathbf{L}^e \left[ \delta \mathbf{E}^e_{\text{trial}} \right] - \frac{\Delta t}{2} \sum_\beta \frac{\partial \dot{\gamma}^\beta}{\partial s^\beta} \left[ \mathbf{L}^e \left[ \mathbf{B}^\beta \right] \otimes \mathbf{S}^\beta_0 \right] \delta \mathbf{T} \\
- \frac{\Delta t}{2} \sum_\beta \frac{\partial \dot{\gamma}^\beta}{\partial \dot{\mathbf{r}}^\beta} \left[ \mathbf{L}^e \left[ \mathbf{B}^\beta \right] \otimes \frac{\partial s^\beta}{\partial \mathbf{T}} \right] \delta \mathbf{T} \\
- \Delta t \sum_\beta \mathbf{L}^e \left[ \mathbf{S}^\beta_0 \mathbf{T} \delta \mathbf{E}^e_{\text{trial}} + \delta \mathbf{E}^e_{\text{trial}} \mathbf{S}^\beta_0 \right] \tag{4.48}
\]

where \( \mathbf{B}^\beta \) is defined in Box 3, \( \frac{\partial \dot{\gamma}^\beta}{\partial s^\beta} \), \( \frac{\partial \dot{\gamma}^\beta}{\partial \dot{\mathbf{r}}^\beta} \) are known from the functional form of \( \dot{\gamma}^\beta \) and \( \delta \mathbf{T} = \mathbf{C} \left[ \delta \mathbf{E}^e_{\text{trial}} \right] \). The tangent moduli are then evaluated as an implicit solution of Equation (4.48). This computation of the tangent moduli requires the evaluation of \( \frac{\partial \mathbf{e}^e}{\partial \mathbf{T}} \), obtained by linearizing Equation (4.40). This linearization (at a
fixed temperature) is given by

\[ \delta s^\alpha = \Delta t \sum_\beta q^{\alpha\beta} \frac{\partial g^\beta}{\partial s^\beta} \delta s^\beta + \Delta t \sum_\beta q^{\alpha\beta} \frac{\partial g^\beta}{\partial T^\beta} \delta T^\beta \] (4.49)

where \( \delta T^\beta = \delta T \cdot S_0^\beta \). An implicit solution of the above equation results in an expression for \( \frac{\partial s^\alpha}{\partial T} \) of the following form:

\[ \frac{\partial s^\alpha}{\partial T} = \sum_\beta m_{\alpha\beta} S_0^\beta \] (4.50)

where \( m_{\alpha\beta} \) is a constant array. The tangent moduli are thus evaluated through Equations (4.48)-(4.50). In all of the above analyses, the standard tensorial notation developed in [45] is followed.

### 4.5 Reduced order model for ODF evolution in an Eulerian framework

In design and control of many complex continuum physical processes, standard simulation techniques using finite elements or spectral methods are not appropriate due to the large number of degrees-of-freedom needed for the analysis and the associated mathematical and computational complexity. It is in this context that reduced-order models play a significant role. These models help reduce the computational complexity by capturing the dynamics of the associated process through smaller number of degrees-of-freedom. The techniques of reduced modeling have been in use for sometime for the control of fluid dynamical systems (see [70]-[74] for applications in turbulence). The proper orthogonal decomposition (POD) technique was first described in [70] and these techniques have since been improved and expanded for mathematical and computational simplicity. Reduced-order modeling involves the development of a reduced set of basis functions, \( \phi_i(\mathbf{r}) \), for the associated
system (represented by a set of partial differential equations). The ODF, \( A(r, t) \), governed by Equation (4.7) is then approximated as:

\[
A(r, t) = \sum_{i=1}^{s} a_i(t) \phi_i(r) \tag{4.51}
\]

and

\[
a_i(t) = \int_R A(r, t) \phi_i(r) dv \tag{4.52}
\]

The optimal basis functions \( \phi_i(r) \), for an accurate representation of the ODF, are generated using the technique of POD (proper orthogonal decomposition) from an ensemble of ODF data, \( \{A^i(r)\}_{i=1}^{N} \), obtained from numerous problem runs. The POD method involves maximizing the average projection of the ensemble data onto the basis. The resulting optimization problem can be mathematically stated as:

\[
\max_{\phi} \frac{\langle (A, \phi) \rangle^2}{\| \phi \|^2} \tag{4.53}
\]

It has been shown [70] that the solution of the problem defined by Equation (4.53), leads to an eigenvalue problem, which can be computationally expensive for large ensembles of ODF data. To reduce the computational effort, the method of snapshots [73] was introduced in which the basis, \( \phi \), is expressed as a linear combination of the original ensemble data as:

\[
\phi_j = \sum_{i=1}^{N} u_j^i A^i \tag{4.54}
\]

where \( u_j^i \) is to be determined such that \( \phi \) maximizes Equation (4.53). The eigenvalue problem then reduces to the following form:

\[
C U = \Lambda U \tag{4.55}
\]

where \( C \) is the spatial correlation matrix and is defined as:

\[
C_{ij} = \frac{1}{N} \int_R A^i(r) A^j(r) dv \tag{4.56}
\]
and $\Lambda$ and $U$ give the complete eigen-description of the system. A suitable basis size, $s$, is computed by maximizing the energy contained by the eigenmodes. The energy contained by the eigenmodes is the sum of the corresponding eigenvalues. Once the modes have been evaluated, Equation (4.51) is used in Equation (4.7) to obtain the following ordinary differential equations (ODEs):

$$\dot{a} = Ba + b \tag{4.57}$$

where $a$ are the time dependent coefficients that determine the ODF and

$$B_{ij} = -\int_{\mathcal{R}} (\nabla \phi_j(r) \cdot \mathbf{v} \phi_i(r) + \phi_j(r) \phi_i(r) \nabla \cdot \mathbf{v}) \, dv \tag{4.58}$$

$$b_i = 0 \tag{4.59}$$

The initial value of $a$ is determined from the initial texture and Equation (4.52) as:

$$a_i(0) = \int_{\mathcal{R}} A(r, t = 0) \phi_i(r) \, dv \tag{4.60}$$

where $A(r, t = 0)$ is the initial texture of the polycrystal. Thus Equations (4.57) – (4.60) define the reduced-order model for the system governed by Equation (4.7).

This is extremely useful in the context of optimal control problems, to obtain a desired orientation distribution function, as only a smaller, finite number of degrees of freedom need to be controlled. It is stressed that the developed reduced-order modeling framework is applicable only in the context of an Eulerian analysis [59].
4.6 Numerical Results

4.6.1 Example 10: Validation of the constitutive model for f.c.c materials (Material point simulator)

In this section, the proposed modeling scheme is validated by comparison with experimental results available in literature. The experimental results [75] of 99.987% pure polycrystalline f.c.c aluminum are used for this purpose. The material properties for this material are provided in Appendix A.5. The numerical experiment simulated a simple shear motion. The initial texturing of the material is assumed to be random, and this corresponds to a constant Lagrangian ODF of 2.435. The reference fundamental region is discretized into 448 tetrahedral elements with cubic symmetry enforced in the solution procedure. The numerical experiments were simulated at a constant strain rate of $6.667 \times 10^{-4} \text{s}^{-1}$ and for temperatures varying from 20K to 300K. The experimental results were obtained by digitizing the stress-strain curves presented in [75]. The predicted and experimental stress-strain responses are superposed in Figure 4.3. Also shown in Figure 4.4 are the reference fundamental region, the deformed fundamental region and the total Lagrangian ODF corresponding to this deformed fundamental region at a plastic strain of 10%. It is observed that the material response is very accurately modeled over a wide range of operating temperatures. The model, however, underpredicts the material response at 20K. Such a response can be attributed to the fact that twinning has not been modeled in this analysis and is known to be prevalent at low temperatures. Additional investigations reveal that this could also be due to the result of a lower saturation value for the slip system resistances. Table 4.1 shows the convergence characteristics of the material point simulator that was obtained in a typical time
Figure 4.3: The material response (equivalent stress strain curve) during a simple shear test for f.c.c Al (Example 10).

step after development of plastic strain. It was observed that the convergence of the solution scheme for the constitutive problem (system described in Box 3) took on average about 4 iterations.

This problem has also been addressed in [8], where a discrete representation of a polycrystal was utilized. It was observed in the analysis of the results that the material point simulator predictions did not accurately model the experimental behavior in [75]. The choice of orientations to make up the sample of discrete orientations and the solution strategy (fully implicit (approach developed in this thesis) versus the mixture of explicit/implicit algorithms used in [8] following the work of [11]) are a few reasons which can significantly affect the performance of the material point simulator. In the present approach however, the continuum description of polycrystals has mitigated the errors from the choice of orientations. It was observed that a coarser finite element discretization of the fundamental region
Figure 4.4: The reference fundamental region, the deformed fundamental region and the corresponding Lagrangian ODF (at plastic strain of about 10%) obtained from the simple shear test of f.c.c Al (Example 10).

<table>
<thead>
<tr>
<th>N-R iteration</th>
<th>Error norm Equation (4.39)</th>
<th>Error norm Equation (4.40)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.5699E-01</td>
<td>2.0565E-02</td>
</tr>
<tr>
<td>2</td>
<td>1.7124E-02</td>
<td>2.5177E-04</td>
</tr>
<tr>
<td>3</td>
<td>6.2980E-04</td>
<td>7.3044E-06</td>
</tr>
<tr>
<td>4</td>
<td>8.3702E-07</td>
<td>9.5333E-09</td>
</tr>
</tbody>
</table>

Table 4.1: Convergence characteristics of the material point simulator at a particular orientation (Example 10).
did not affect the performance and accuracy of the material point simulator. In particular, the computed results were only slightly different from the results in Fig. 4.4 when using a discretization of 68 tetrahedral elements instead of 448 for the reference fundamental region, whereas removing certain orientation descriptions from the sample of discrete orientations will severely affect the performance and accuracy of the materials point simulator.

Similar detailed studies were performed for b.c.c Tantalum and the results are reported in [60]. Based on these results, it is concluded that the developed continuum analysis is more accurate and reliable than the discrete analysis available in literature. It is also observed that the framework developed here is able to accurately capture the behavior of both b.c.c and f.c.c materials.

4.6.2 Example 11: Open die forging problem using thermo-elasto viscoplasticity

The upset forging of a cylindrical billet (of f.c.c Aluminium) between parallel flat dies is considered as an introductory application of the developed Lagrangian model towards a large deformation metal forming problem. Figure 4.5 presents a schematic of the problem. In this forging simulation, the initial cylindrical billet is 2 mm in diameter and 2 mm high. The forging die is modeled as a rigid surface and to simulate sticking friction between the die and workpiece, a coefficient of friction of 0.4 is applied. The deformation is highly non-homogeneous with variable rates of straining at material points and time varying contact. The symmetry of the problem allowed modeling one eighth of the geometry. A nominal strain rate of $10^{-2}/s$ was applied during the forging process. A very coarse grid of 24 brick elements was used to discretize the domain. The reference fundamental region at each of the material
points is discretized through 448 tetrahedral elements. The initial microstructure is assumed to be random, thus a random ODF is considered as the reference ODF. This initial billet was subject to a height reduction of 15% at a fixed time step of 0.01 s, at a fixed forging rate of 0.01 sec\(^{-1}\). The material properties are described in Appendix A.5. The initial temperature of the billet is assumed to be uniform and equal to 300\(^\circ\)K. Figure 4.6 shows the contours of the equivalent stress and temperature after 15% deformation. The deformed fundamental region and the Lagrangian ODF (texture) at the center of the workpiece are described in Figure 4.7.

This region is associated with a purely compressive deformation during the forging process and this can be verified from the ODF which describes the texture obtained for f.c.c materials under uniaxial compression. The force necessary to forge the workpiece with increasing stroke is documented in Figure 4.8. The computa-
Figure 4.6: The contours of equivalent stress and temperature during flat die forging of a cylindrical billet made of f.c.c Al (Example 11).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time</td>
<td>150:12:46 (hr:min:sec format)</td>
</tr>
<tr>
<td>Contact augmentation per iteration</td>
<td>2</td>
</tr>
<tr>
<td>Average N-R iterations/time step</td>
<td>3</td>
</tr>
<tr>
<td>Formation of the linear system</td>
<td>250 s</td>
</tr>
</tbody>
</table>

Table 4.2: Computing statistics for the open die forging of a cylindrical billet (Example 11). Contact augmentation is defined in the contact algorithm in [37].

<table>
<thead>
<tr>
<th>Iteration number</th>
<th>Displacement error norm</th>
<th>Energy error norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.6951E-02</td>
<td>1.000E+00</td>
</tr>
<tr>
<td>2</td>
<td>5.7735E-04</td>
<td>6.281E-02</td>
</tr>
<tr>
<td>3</td>
<td>2.3790E-06</td>
<td>4.6638e-06</td>
</tr>
</tbody>
</table>

Table 4.3: Macro-problem convergence characteristics in a typical time step for the open die forging of a cylindrical billet (Example 11). The convergence characteristics of the micro-problem were presented in Table 4.1.
4.6.3 Example 12: Material point simulator in an Eulerian framework - Comparing reduced-order model with full-order model

A uniaxial tension test is conducted on a polycrystal made of f.c.c Copper. The material properties and constitutive models for this framework are detailed in [19].
Figure 4.8: The upsetting force versus die stroke during flat die forging of a cylindrical billet made of f.c.c Al (Example 11).

The velocity gradient is defined as

\[
\begin{bmatrix}
1.0 & 0.0 & 0.0 \\
0.0 & -0.5 & 0.0 \\
0.0 & 0.0 & -0.5
\end{bmatrix}
\]  \hspace{2cm} (4.61)

An Eulerian analysis was performed, similar to that in [19], and the ODFs developed using the full-order model and the reduced-order model, at a plastic strain of 20%, are compared in Figure 4.9. The reduced-order basis was generated from the data of different uniaxial deformation processes. Postprocessing indicates that the $L_2$ norm of the error was about 3.4% of the random ODF. The maximum value of the ODF’s from the full-order model was 7.4 and that from the reduced-order model was 7.2. Furthermore, the maxima and minima were observed at the same locations in both the full-order and reduced-order solutions. The reduced-order model consisted of only 3 modes while there were 145 degrees-of-freedom in the full-order model. The overall speed up of the material point simulator was found to be around 6 without any appreciable loss of accuracy. The numerous examples, detailed in [58, 59], have
shown that the developed reduced-order modeling approach works well not only in the interpolatory mode but also in the extrapolatory mode with only a few basis functions.
Chapter 5

Multi-length scale continuum sensitivity analysis

In the previous chapter, a multi-length scale approach was developed to accurately model the behavior and response of polycrystalline materials. The framework developed in Chapter 4 is extended to address optimization problems for these materials. In order to develop a gradient based optimization framework for polycrystalline materials, a multi-length scale continuum sensitivity analysis has to be developed. The next few sections address the development of an innovative sensitivity analysis and some exploratory examples of design problems.

5.1 Deformation sensitivity problem

The definitions for sensitivity fields, discussed in Chapter 3, are extended towards a multi-length scale framework. The process of evaluating the sensitivities of fields on the micro-scale due to perturbations on the macro-scale is shown schematically in Figure 5.1. This requires a macro-sensitivity problem where the interest is to
Figure 5.1: Pictorial of the two-length scale sensitivity analysis. On the left, the macro-sensitivity problem (following a Lagrangian approach) computes the sensitivities of continuum fields (e.g. of the velocity gradient) with respect to macro-design variables (here the die surface). On the right, the micro-sensitivity problem (following an Eulerian approach) computes the sensitivity of the ODF and properties related to the ODF.

compute how perturbations on the macro-design variables $\beta$ affect the continuum fields - the deformation gradient $F$ and the velocity gradient $L$. This macro-sensitivity problem was examined in detail in Chapter 3. The dependence of the deformation gradient $F$ on $\beta$, in a total Lagrangian framework, can be expressed as $F = F(\mathbf{X}, t; \beta)$. The parameter sensitivity $\frac{\partial}{\partial \beta} F(\mathbf{X}, t; \beta, \Delta \beta)$ is defined as the total Gateaux differential of the deformation gradient in the direction $\Delta \beta$ computed
at $\beta$:
\[
\overset{\circ}{F}(X, t; \beta, \Delta \beta) = \left. \frac{d}{d\lambda} F(X, t; \beta + \lambda \Delta \beta) \right|_{\lambda=0} (5.1)
\]

The micro-sensitivity problem, also defined in Figure 5.1, computes the resulting variation of the ODF and other microstructural properties from the perturbation $\Delta F$ of $F$ (or $\Delta L$ of the velocity gradient $L$). In extending the direct analysis in Chapter 4, which was based on the Taylor hypothesis, Taylor hypothesis for a sensitivity problems is developed.

The Taylor hypothesis for the sensitivity analysis is defined as follows: **the sensitivity of the deformation gradient at a material point is taken to be the same as the sensitivity of the deformation gradient of the underlying crystals, in the sample reference frame.**

This is used extensively in developing the constitutive sensitivity analysis for a single crystal. For the material point simulator developed here, a design vector $\beta$ on the micro-scale is defined such that it has a one-to-one relation with $F$. The salient feature of such an approach is that equations governing the sensitivity fields are computed at the continuum level in all length scales. The equilibrium equation is considered and design differentiated. This continuum, differential, sensitivity equilibrium equation is then posed in a weak form so as to establish a principle of virtual work like equation for the calculation of the sensitivity of deformation fields. Consistent with this mode of analysis, the sensitivity constitutive and sensitivity thermal are derived from their corresponding continuum equations rather than their numerically integrated counterparts.

Before the sensitivity problems are discussed, the polycrystal average of sensitivity fields needs to be defined. Based on our earlier definition (in Chapter 4, for the polycrystal average of an orientation dependent property, $Y(r, t; \beta)$), the polycrystal
average of the corresponding sensitivity field is determined as follows

\[
\langle \dot{\Upsilon} \rangle = \frac{\int_{\mathcal{R}_t} \Upsilon(r, t; \beta) A(r, t; \beta) \, dv_t}{\mathcal{R}_t}
\]

\[
= \int_{\mathcal{R}} \dot{\Upsilon}(s, t; \beta) A_0(s) \, dv
\]

(5.2)

where \( dv_t \) is defined as the volume element on the current fundamental region and it is assumed that the initial texture is fixed (i.e. \( A_0 = 0 \)). From Equation (5.2), one can conclude that at no point in the analysis, the sensitivity of the ODF is needed to compute the polycrystal average of different properties. Examples discussed later in this Chapter, however, do report the sensitivity of the ODF as a post-processing step for validating the developed analysis.

Described below is the analysis for the development of a total Lagrangian sensitivity formulation for the kinematic problem. Let the reference configuration be \( B_0 \). The design differentiation of the equilibrium equation (Equation 2.8) results in:

\[
\dot{\nabla}_0 \cdot \langle \dot{P} \rangle + \dot{f} = 0
\]

(5.3)

where \( \langle \dot{P} \rangle \) is the polycrystal averaged PK-I stress defined in earlier chapters. A variational form for the sensitivity equilibrium equation (for parameter sensitivity) can be posed as follows: Evaluate \( \tilde{x} = \hat{x}(X, t; \beta, \Delta \beta) \) such that [50]

\[
\int_{\mathcal{B}_0} \dot{\nabla}_0 \tilde{\eta} dV_0 = \int_{\partial \mathcal{B}_0} \dot{\lambda} \cdot \tilde{\eta} \, dA_0
\]

(5.4)

for every \( \tilde{\eta} \), a kinematically admissible sensitivity deformation field expressed over the reference configuration \( \mathcal{B}_0 \). In order to solve the weak form, defined by Equation (5.4), relationships between (a) \( \dot{F} \) and \( \tilde{x} \) \( \langle \dot{P} \rangle \) and \( [\dot{F}, \tilde{\theta}] \) and (c) \( \dot{\lambda} \) and \( \tilde{x} \) need to be developed. The relationship between \( \dot{F} \) and \( \tilde{x} \) is purely kinematic and has been described in Chapter 3. The relationship between \( \langle \dot{P} \rangle \) and \( [\dot{F}, \tilde{\theta}] \) is obtained
from the sensitivity constitutive problem to be discussed in Section 5.2 and takes the form:

\[
\langle \overset{\circ}{P} \rangle = \mathcal{B} \left[ \overset{\circ}{F} \right] + A \overset{\circ}{\theta} + B
\]  

(5.5)

where \( \mathcal{B} \) is a fourth order tensor and \( A, B \) are second order tensors. These tensors, are constants, defined from known direct and sensitivity fields at the previous time step, and are obtained by considering the polycrystal average of each crystal response (see Section 5.2). The constitutive sensitivity analysis for a single crystal is similar to the analysis developed for phenomenological models in Chapter 3. The relationship between \( \overset{\circ}{\lambda} \) and \( \overset{\circ}{x} \) is obtained from the sensitivity contact problem as \( \overset{\circ}{\lambda} = H[\overset{\circ}{x}] + d \), where \( H \) is a second order tensor and \( d \) a vector. The non-trivial derivation of these tensors resulting by design-differentiation of a regularized contact problem can be found in [41].

### 5.2 Sensitivity constitutive problem

Through the crystal sensitivity constitutive sub-problem, the relationship between the polycrystal average, \( \langle \overset{\circ}{T} \rangle \) and \( \{ \overset{\circ}{F}, \overset{\circ}{\theta} \} \) is computed. As part of the update procedure, one computes the set \( \{ \overset{\circ}{T}, \overset{\circ}{s}, \overset{\circ}{\tau}, \overset{\circ}{F}^e, \overset{\circ}{F}^p \} \) for each crystal orientation at the end of the time increment \( t_{n+1} \), where the sensitivity of the total deformation gradient \( \overset{\circ}{F}_{n+1} \) and the sensitivity of the temperature field \( \overset{\circ}{\theta}_{n+1} \) are assumed known.

The polycrystal average of \( \overset{\circ}{W}_{\text{mech}} \), sensitivity of the mechanical dissipation \( W_{\text{mech}} \), is also computed as being a driving force for the thermal sensitivity problem at time \( t_{n+1} \) (refer to [54]). The solution of the direct thermo-mechanical problem is known at time \( t_{n+1} \), the body configuration \( \mathcal{B}_{n+1} \) as well as the temperature field \( \theta_{n+1} \) are known at \( t_{n+1} \). The constitutive sensitivity problem for a crystal orientation is his-
tory dependent and the solution of the sensitivity problem at time \( t_n \) is assumed known for each crystal orientation, yielding the variables \( \{\overset{\circ}{T}, \overset{\circ}{s}, \overset{\circ}{\tau}, \overset{\circ}{F}^e, \overset{\circ}{F}^p\} \) at the beginning of each time increment. It was also described in Chapter 3, that the deformation sensitivity response is dependent only on the instantaneous temperature sensitivity response \( \overset{\circ}{\theta}_{n+1} \).

### 5.2.1 Computing the linear relation between \( \overset{\circ}{s}^\alpha \) and \( \{\overset{\circ}{T}_{n+1}, \overset{\circ}{\theta}_{n+1}\} \)

Consider the design-differentiation of the evolution equation for the deformation resistance, \( s^\alpha \) (Equation 4.25). It results in:

\[
\frac{\partial \overset{\circ}{s}^\alpha}{\partial t} = \sum_\beta \left[ h^{\alpha\beta} \dot{\gamma}^\beta + h^{\alpha\beta} \overset{\circ}{\gamma}^\beta \right]
\]  

(5.6)

Incorporating Equations (4.26) and (4.27) and performing an Euler-backward integration results in:

\[
\begin{align*}
\overset{\circ}{s}^\alpha_{n+1} - \Delta t \sum_\beta q^{\alpha\beta} \frac{\partial g^\beta}{\partial s^\beta} \overset{\circ}{s}^\beta_{n+1} = & \overset{\circ}{s}^\alpha_n + \\
\Delta t \sum_\beta q^{\alpha\beta} \frac{\partial g^\beta}{\partial \tau^\beta} \overset{\circ}{\tau}^\beta_{n+1} + \Delta t \sum_\beta q^{\alpha\beta} \frac{\partial g^\beta}{\partial \theta} \overset{\circ}{\theta}_{n+1} 
\end{align*}
\]  

(5.7)

Solving the above set of equations for \( \overset{\circ}{s}^\alpha_{n+1} \) results in:

\[
\overset{\circ}{s}^\alpha_{n+1} = \sum_\beta m^{\alpha\beta} \overset{\circ}{\tau}^\beta_{n+1} + v_1^\alpha \overset{\circ}{\theta}_{n+1} + v_2^\alpha
\]  

(5.8)

where \( m^{\alpha\beta}, v_1^\alpha \) and \( v_2^\alpha \) are constants. It is further known that \( \tau^\beta = \overset{\circ}{T} \cdot \overset{\circ}{S}^\alpha_0 \); design-differentiation of this relation results in \( \overset{\circ}{\tau}^\beta = \overset{\circ}{T} \cdot \overset{\circ}{S}^\alpha_0 \). Note that \( \overset{\circ}{S}^\alpha_0 \) is a constant as it is expressed in the plastically deformed configuration which has the same crystal orientation as in the reference configuration. Substituting this relation into Equation (5.8) results in the desired linear relation:

\[
\begin{align*}
\{\overset{\circ}{s}_{n+1}\} = & \left[ \frac{Ds}{D\tau} \right] : \overset{\circ}{T} + \{v_1\} \overset{\circ}{\theta} + \{v_2\} 
\end{align*}
\]  

(5.9)

where \( \left[ \frac{Ds}{D\tau} \right] \) is a 3\textsuperscript{rd} order tensor and \( v_1, v_2 \) are vectors.
5.2.2 Computing the linear relation between
\[ F_{n+1}^p \text{ and } \{ \bar{T}_{n+1}, \bar{\theta}_{n+1} \} \]

The evolution equation for \( F^p \) is evaluated, by design differentiating Equation 4.13, as:
\[ \frac{\partial F^p}{\partial t} = \bar{L}^p F^p + \bar{F}^p F^p \]  (5.10)
where \( \bar{L}^p = \sum_\alpha \left[ \hat{\gamma}^\alpha S_0^\alpha \right] \) can be computed as,
\[ \bar{L}^p = \sum_\alpha \left[ \frac{\partial \hat{\gamma}^\alpha}{\partial \tau^\alpha} \tau^\alpha + \frac{\partial \hat{\gamma}^\alpha}{\partial s^\alpha} s^\alpha + \frac{\partial \hat{\gamma}^\alpha}{\partial \theta} \theta \right] S_0^\alpha \]  (5.11)
Euler-backward integration of Equation (5.10), with Equations (5.9), (5.11) and the earlier definition of \( \tau^\alpha \) results in the following:
\[ F_{n+1}^p(F_{n+1}^p)^{-1} = E + \mathcal{F} \bar{T}_{n+1} + G \bar{\theta}_{n+1} \]  (5.12)
where \( E, G \) are constant second-order tensors and \( \mathcal{F} \) is a fourth-order tensor. Furthermore, \( \bar{T}_{n+1} \) is related to \( F_{n+1}^e \) and \( \bar{\theta}_{n+1} \) as (by design differentiating Equation (2.6)):
\[ \bar{T} = \left( \frac{\partial \mathcal{L}^e}{\partial \theta} \right) [E^e] \bar{\theta} + \mathcal{L}^e \left[ \text{Sym} \left( F^e T F^e \right) \right] \]  (5.13)
where \( \mathcal{L}^e \), the fourth-order anisotropic elasticity tensor, is assumed to be a function of temperature only. Using Equations (5.12) and (5.13), one can further obtain \( F_{n+1}^p(F_{n+1}^p)^{-1} \) as a function of \( F_{n+1}^e \) and \( \bar{\theta}_{n+1} \).

5.2.3 Computing the linear relation between
\[ F_{n+1}^e \text{ and } \{ F_{n+1}, \bar{\theta}_{n+1} \} \]

Starting from the multiplicative decomposition of the deformation gradient, one can write \( F_{n+1} = F_{n+1}^e F_{n+1}^p + F_{n+1}^e F_{n+1}^p, \) which can then be simplified to,
\[ \left( F_{n+1}^e \right)^{-1} \left( F_{n+1} \right) F_{n+1} = \left( F_{n+1}^e \right)^{-1} F_{n+1}^e + \bar{F}_{n+1} \left( F_{n+1}^p \right)^{-1} \]  (5.14)
Substitution of the linear relationship between $\mathbf{F}_{n+1}^p$ and $[\mathbf{F}_{n+1}, \theta_{n+1}]$ results in the desired linear relationship:

$$\mathbf{F}_{n+1}^e = C' (\mathbf{V}_{n+1}) \begin{bmatrix} \mathbf{F}_{n+1} \end{bmatrix} + \mathbf{H} (\mathbf{V}_{n+1}, \mathbf{V}_n) + \mathbf{M} (\mathbf{V}_{n+1}) \theta_{n+1}$$ (5.15)

where $\mathbf{H}$ and $\mathbf{M}$ are known second order tensor functions and $C'$, a known fourth order tensor function. The relationship between $\mathbf{T}_{n+1}$ and $[\mathbf{F}_{n+1}, \theta_{n+1}]$ is obtained by design differentiating Equation (4.18):

$$\mathbf{T} = -\frac{\text{tr} \left( \mathbf{F}^e (\mathbf{F}^e)^{-1} \right)}{\det(\mathbf{F}^e)} \mathbf{T} + \frac{1}{\det(\mathbf{F}^e)} \mathbf{F}^e \mathbf{T} \mathbf{F}^e^T + \frac{1}{\det(\mathbf{F}^e)} \mathbf{F}^e^T \mathbf{F}^e^T$$ (5.16)

Substitution of the linear relation between $\mathbf{F}_{n+1}^e$ and $[\mathbf{F}_{n+1}, \theta_{n+1}]$ in Equation (5.16), results in a linear relation between $\mathbf{T}_{n+1}$ and $[\mathbf{F}_{n+1}, \theta_{n+1}]$.

The previous sections dealt with finding linear relations between various sensitivity terms for a given crystal orientation. This analysis has to be performed at all orientations to compute the polycrystal average. Consider, for example, the sensitivity of PK-I stress:

$$\langle \mathbf{P} \rangle = \left\langle \left[ \text{tr} \left( \mathbf{F} \mathbf{F}^{-1} \right) \det \mathbf{F} \mathbf{T} \mathbf{F}^{-T} + \det \mathbf{F} \mathbf{T} \mathbf{F}^{-T} - \det \mathbf{F} \mathbf{T} \mathbf{F}^{-T} \mathbf{F} \mathbf{T} \mathbf{F}^{-T} \right] \right\rangle$$

$$= \text{tr} \left( \mathbf{F} \mathbf{F}^{-1} \right) \det \mathbf{\langle T \rangle} \mathbf{F}^{-T} + \det \mathbf{\langle T \rangle} \mathbf{F}^{-T} - \det \mathbf{\langle T \rangle} \mathbf{\mathbf{F}^{-T} \mathbf{T} \mathbf{F}^{-T}}$$ (5.17)

where $\langle \mathbf{T} \rangle = \int_{\mathcal{R}_0} \mathbf{T} A_0 dv$ and $\mathbf{T}$ is described by the relations developed earlier. From these equations, one can generate the constants in Equation (5.5) and use this in the solution of the sensitivity kinematic problem.
5.2.4 Post-processing step: calculating the sensitivity of the spin vector, $\overset{\circ}{\omega}$

Once $\overset{\circ}{F}_{n+1}^e$ has been evaluated from the previous sub-sections, $\overset{\circ}{R}_{n+1}^e$ can be obtained as \[\text{[36]}\] (subscript $n + 1$ is dropped in this Equation):

$$\overset{\circ}{R}_e = \overset{\circ}{F}_e \overset{\circ}{F}_e^{-1} \overset{\circ}{R}_e - \overset{\circ}{R}_e^{\text{sym}} \left\{ U_e^{\text{sym}} \left( F_e^T \overset{\circ}{F}_e \right) \right\} F_e^{-1} R_e$$  \hspace{1cm} (5.18)

From Chapter 4, it is also known that $\omega$, which represents the spin vector, is defined as

$$\omega = \text{vect}(\overset{\circ}{\Omega}) = \text{vect}(\Omega)$$  \hspace{1cm} (5.19)

where $R_e$ is evaluated through the polar decomposition of the elastic deformation gradient $F_e$, as $F_e = R_e U_e$, and $\Omega$, the spin tensor, is defined as:

$$\Omega = \overset{\circ}{R}_e R_e^T$$  \hspace{1cm} (5.20)

Design differentiating Equations (5.19) and (5.20), the sensitivities of the corresponding quantities is obtained as:

$$\overset{\circ}{\omega} = \text{vect}(\overset{\circ}{\Omega})$$  \hspace{1cm} (5.21)

$$\overset{\circ}{\Omega} = \overset{\circ}{R}_e R_e^T - \Omega \overset{\circ}{R}_e R_e^T$$  \hspace{1cm} (5.22)

where $\overset{\circ}{R}_e^{\text{sym}} = - R_e^T \overset{\circ}{R}_e R_e^T$. Euler-backward integration of Equation 5.22 results in (refer to Appendix B.1 for the time integration procedure):

$$\overset{\circ}{\Omega} = \frac{1}{\Delta t} \left[ \overset{\circ}{R}_e R_e^T - R_e R_e^T_n \overset{\circ}{R}_e R_e^T_n \right]$$  \hspace{1cm} (5.23)

where the subscript $(n + 1)$ has been dropped for convenience and $\overset{\circ}{R}_e$ was evaluated in Equation (5.18). Further, $\overset{\circ}{\omega}$ can be evaluated from Equation (5.21).
5.3 Sensitivity analysis of the orientation distribution function

5.3.1 Analysis in a Lagrangian framework

Consider the re-orientation velocity defined in Equation (4.35). The design-differentiation of this equation results in the sensitivity of the re-orientation velocity:

\[
\vec{v} = \frac{\partial \vec{r}}{\partial t} = \frac{1}{2} \left[ \vec{\omega} + (\vec{\omega} \cdot \vec{r}) \vec{r} + \vec{\omega} \times \vec{r} \right] + \frac{1}{2} [\omega \otimes r + (\omega \cdot r) I + \Omega] \vec{r}
\]

which can further be written as

\[
\frac{\partial \vec{r}}{\partial t} - M_2 \vec{r} = \frac{1}{2} \left( \vec{\omega} + (\vec{\omega} \cdot \vec{r}) \vec{r} + \vec{\omega} \times \vec{r} \right)
\]

where \( M_2 = \frac{1}{2} \{\omega \otimes r + (\omega \cdot r) I + \Omega\} \) and \( \vec{\omega} \) was defined in the previous section.

Assuming small time steps and applying an Euler-backward time integration scheme, leads to the following linear system (refer to Appendix B.2 for the time integration procedure):

\[
\vec{r}_{n+1} = \left\{ I + \frac{\Delta t}{2} \{ \omega_{n+1} \otimes r_{n+1} + (\omega_{n+1} \cdot r_{n+1}) I + \Omega_{n+1} \} \right\} r_n + \frac{\Delta t}{2} \left[ \omega_{n+1} + (\omega_{n+1} \cdot r_{n+1}) r_{n+1} + \omega_{n+1} \times r_{n+1} \right]
\]

which can be solved for \( \vec{r}_{n+1} \) to compute sensitivity of the current fundamental region.

Now consider the Lagrangian version of the ODF conservation equation (Equation (4.6)). Design differentiation of this equation, assuming that the initial texture is independent of the design parameters, leads to the following:

\[
\dot{\hat{A}}(s, t; \beta, \Delta \beta) J(s, t; \beta) = -\hat{A}(s, t; \beta) \hat{J}(s, t; \beta, \Delta \beta)
\]
where \( J(s, t; \beta, \Delta \beta) = \det(\nabla \hat{r}(s, t; \beta, \Delta \beta)) = -J(s, t; \beta) \left[ \nabla \cdot \hat{r}(s, t; \beta, \Delta \beta) \right] \) [45] and \( \hat{r} \) has been evaluated in Equation (5.26).

### 5.3.2 Analysis in an Eulerian framework

The sensitivity problem, corresponding to the evolution of the ODF in an Eulerian framework, discussed in Chapter 4, is developed in this section. The sensitivity of the Eulerian ODF is denoted by \( \hat{A} = \hat{A}(r, t; \beta, \Delta \beta) \). Using the earlier definition of parameter sensitivity, design differentiation of Equation (4.7) results in the following partial differential equation:

\[
\frac{\partial \hat{A}}{\partial t} + \nabla \hat{A} \cdot \hat{v} + \nabla \hat{A} \cdot \hat{v} + \hat{A} \nabla \cdot \hat{v} + \hat{A} \nabla \cdot \hat{v} = 0 \quad (5.28)
\]

where the sensitivity of the re-orientation velocity is:

\[
\hat{v} = \frac{\partial \hat{r}}{\partial t} = \frac{1}{2} \left[ \hat{\omega} + (\hat{\omega} \cdot r) r + \hat{\omega} \times r \right] \quad (5.29)
\]

where \( \hat{\omega} \) has been evaluated in the sensitivity constitutive problem.

**Remark 1:** Equations (5.24) and (5.29) clearly highlight how the sensitivity of the re-orientation velocity differ for Lagrangian and Eulerian analysis. In the Eulerian analysis, the orientation parameterization, \( r \), does not depend on the design parameter (macroscopic or microscopic) \( \beta \), whereas in the Lagrangian analysis, the deforming fundamental region depends strongly on \( \beta \).

From Equation (5.28), a weak formulation, for the sensitivity of the ODF, over the fundamental region follows as:

\[
\int_{\mathcal{R}} \left( \frac{\partial \hat{A}}{\partial t} + \nabla \hat{A} \cdot \hat{v} + \nabla \hat{A} \cdot \hat{v} + \hat{A} \nabla \cdot \hat{v} + \hat{A} \nabla \cdot \hat{v} \right) \varphi dv = 0 \quad (5.30)
\]

where \( \varphi \) is an admissible test function. Detailed discussions of the solution process, to compute the sensitivities, can be found in [59].
5.3.3 Reduced-order models for the sensitivity ODF problem in an Eulerian framework

Computational design of multi-length scale deformation problems can be simplified through the development of a reduced-order model for the sensitivity problem. The reduced-order model for the sensitivity problem is obtained from the basis developed for the direct problem (Section 4.5). The sensitivity of the ODF field is approximated in terms of the basis functions as:

\[
\begin{aligned}
\hat{\mathbf{A}}(\mathbf{r}, t) &= \sum_{i=1}^{s} c_i(t) \phi_i(\mathbf{r}) \\
c_i(t) &= \int_{\mathcal{R}} \hat{\mathbf{A}}(\mathbf{r}, t) \phi_i(\mathbf{r}) \, d\mathbf{v}
\end{aligned}
\] (5.31)

and

\[
\begin{aligned}
\dot{c}_i &= G_{ij} c_j + h_i
\end{aligned}
\] (5.33)

where \(c\) is the time dependent coefficient that determines the sensitivity ODF field and the choice of \(s\) was discussed in Section 4.5. Performing an analysis similar to that in the direct problem, the reduced system is obtained as:

\[
\begin{aligned}
\dot{c} &= Gc + h
\end{aligned}
\] (5.33)

where

\[
\begin{aligned}
G_{ij} &= -\int_{\mathcal{R}} (\nabla \phi_j \cdot \mathbf{v} \phi_i + \phi_j \phi_i \nabla \cdot \mathbf{v}) \, d\mathbf{v} \\
h_i &= -\int_{\mathcal{R}} \left( \nabla \mathbf{A} \cdot \hat{\mathbf{v}} \phi_i + \mathbf{A} \phi_i \nabla \cdot \hat{\mathbf{v}} \right) \, d\mathbf{v}
\end{aligned}
\] (5.34, 5.35)

and \(\mathbf{A}\) is the Eulerian ODF field obtained from the direct problem in Chapter 4. The initial value of \(c\), when \(\hat{\mathbf{A}}(\mathbf{r}, t = 0) = 0\) is assumed, is obtained from Equation (5.32) as:

\[
\begin{aligned}
c_i(0) &= \int_{\mathcal{R}} \hat{\mathbf{A}}(\mathbf{r}, 0) \phi_i(\mathbf{r}) \, d\mathbf{v} = 0
\end{aligned}
\] (5.36)
5.4 Validation of the sensitivity analysis

5.4.1 Example 13: Validating the sensitivity algorithm in an Eulerian framework

An accuracy study is performed for the ODF sensitivity solutions obtained from the full-order and reduced-order models for the Eulerian sensitivity analysis developed in the earlier section. This problem is based on the direct problem discussed in Section 4.6.3. In addition to comparing the solutions of the full- and reduced-order models, the accuracy of the sensitivity fields are validated by comparison with the sensitivity obtained from the forward finite difference method (FDM). The finite difference sensitivities are computed in the same method as that highlighted in Chapter 3. The continuum sensitivity analysis was performed on f.c.c Copper about the reference direct problem described in Section 4.6.3. The material parameters and constitutive models are described in [19]. The design velocity gradient is given as

\[
L = \begin{bmatrix}
1.0 & 0.0 & 0.0 \\
0.0 & -0.5 & 0.0 \\
0.0 & 0.0 & -0.5 \\
\end{bmatrix}
\]  

(5.37)

The perturbation to the velocity gradient is given by (1% perturbation to \(L\)):

\[
\Delta L = \begin{bmatrix}
0.01 & 0.0 & 0.0 \\
0.0 & -0.005 & 0.0 \\
0.0 & 0.0 & -0.005 \\
\end{bmatrix}
\]  

(5.38)

The reference ODF’s, obtained from the full-order and reduced-order models, at a plastic strain of 20% are shown in Figure 4.9. The sensitivity of the ODF is evaluated through 3 different methods: forward-based finite difference approximation (FDM),
full-order model and reduced-order model (with the same basis as in Section 4.6.3). The sensitivity results obtained from these methods are compared in Figure 5.2. It was observed that the $L_2$ norm of the error for the full-order model (with respect to the FDM solution) was 6% of the maximum FDM solution. Similar analysis performed on the reduced-order model resulted in an error of about 10%. Further, it was observed that the maxima and minima of the sensitivity field were under-predicted by the reduced-order modeling approach even though the distributions remained similar to that of the full-order model. It was also observed that as the number of basis functions increased, the quality of the solution approached the full-order model solution. More details about the convergence of the solution with increasing basis functions can be obtained from [58].

5.4.2 Gradient based optimization: Process design for desired ODF

The design problem discussed here is based at a material point. As part of the solution process, macroscopic control parameters $\beta$ are chosen such that it leads to a desired distribution of a micro-field $\Upsilon$. This micro-field is assumed to be the ODF in the optimization examples discussed below. Examples of process control for other mechanical and magnetic properties are discussed in [58, 59]. The control problem is posed as an optimization problem with the objective function stated as:

$$
\min_{\beta} \mathcal{F}(\beta) = \frac{1}{N_s} \sum_{i=1}^{N_s} (A_i(\beta) - A^\text{desired}_i)^2
$$

(5.39)

where $N_s$ is the number of sampling points. The sampling points correspond to specific orientations in the fundamental region and $A^\text{desired}$ is a discrete representation of the desired texture.
Figure 5.2: Comparison of the sensitivity of the ODF obtained using the full-order model, the corresponding reduced-order model and FDM solution at the final time (t = 0.20 seconds) for a uniaxial tension test (Example 13 - Polycrystal sensitivity analysis for f.c.c Copper).
The optimization process consists of computing the gradients of various Lagrangian or Eulerian fields $\Upsilon$ that are represented as: $\nabla \Upsilon = \left( \frac{\partial \Upsilon}{\partial \beta_1}, \frac{\partial \Upsilon}{\partial \beta_2}, \ldots, \frac{\partial \Upsilon}{\partial \beta_n} \right)$. These gradients are evaluated from continuum sensitivity fields $\hat{\Upsilon}$ as (refer Section 3.6.1):

$$\frac{\partial \Upsilon}{\partial \beta_i} = \frac{\hat{\Upsilon}(\mathbf{r}, t; \beta_1, \beta_2, \ldots, \beta_n, 0, \ldots, 0, \Delta \beta_i, 0, \ldots, 0)}{\Delta \beta_i} \quad (5.40)$$

The evaluation of the gradient requires $n$ continuum sensitivity problems where the $i^{th}$ sensitivity problem is driven by $\Delta \beta_i$ with $\Delta \beta_j = 0$ for $j \neq i$. Thus, for computing the sensitivity fields one nonlinear direct problem and $n$ linear sensitivity problems are needed (a total of $n + 1$ problems). In comparison, the finite difference method (FDM) needs solution to $n + 1$ nonlinear direct problems to evaluate $\nabla \Upsilon$. The problem definition considers the entire range of permissible control parameters (i.e. largest possible solution space) thus guaranteeing the existence of a solution. The gradient optimization methodology results in a local minimum and other heuristic optimization techniques need to be considered if interested in a global solution.

Owing to the highly non-linear nature of the objective function, step size control must be exercised to achieve monotonic convergence. The next section highlights particular applications of the developed algorithms.

5.4.3 Example 14: Eulerian analysis - design for a desired ODF using full-order model

The macroscopic design parameter is assumed to be the velocity gradient $L$. Therefore, this problem deals with the design/control of the velocity gradient to obtain a desired orientation distribution function (ODF), with the objective function defined in Equation (5.39). The problem statement is as follows: given a desired ODF distribution - which translates to a desired property distribution - determine the velocity
gradient, obtained from the full-order model, was computed as: described by the objective function in Figure 5.5. The converged (optimal) velocity plastic strain, is shown in Figure 5.4. The progress of the optimization problem is shown in Figure 5.3. The ODF obtained through the optimal process, at 20% The initial guess to the design problem was zero velocity gradient, i.e., as:

\[
L = \beta_1 \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & -0.5 & 0.0 \\ 0.0 & 0.0 & -0.5 \end{bmatrix} + \beta_2 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & -1.0 \end{bmatrix} + \beta_3 \begin{bmatrix} 0.0 & 1.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} + \\
+ \beta_4 \begin{bmatrix} 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} + \beta_5 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix} + \beta_6 \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix} + \\
+ \beta_7 \begin{bmatrix} 0.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} + \beta_8 \begin{bmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -1.0 \\ 0.0 & 1.0 & 0.0 \end{bmatrix}
\] (5.41)

The desired ODF was originally obtained through a velocity gradient represented as:

\[
\beta_{actual} = \{1, 0, 0.866, 0, 0, 0, 0, 0\}
\] (5.42)

The initial guess to the design problem was zero velocity gradient, i.e.,

\[
\beta_{guess} = \{0, 0, 0, 0, 0, 0, 0, 0\}
\] (5.43)

The desired ODF and the ODF obtained from the initial guess at 20% strain is shown in Figure 5.3. The ODF obtained through the optimal process, at 20% plastic strain, is shown in Figure 5.4. The progress of the optimization problem is described by the objective function in Figure 5.5. The converged (optimal) velocity gradient, obtained from the full-order model, was computed as:

\[
\beta_{optimal} = \{0.962, 0, 0.867, 0, 0, 0, 0, 0\}
\] (5.44)
Figure 5.3: The ODF’s involved in the full-order optimization problem. Shown are the desired ODF and the ODF obtained from the initial guess for the process solution (Example 14).

5.4.4 Example 15: Eulerian analysis - design for a desired ODF using reduced-order model

The design problem described in Section 5.4.3 was repeated using the reduced-order model for the direct and sensitivity analysis. The reduced basis was selected from snapshots taken during deformation problems consisting of shear, tension and plane
Figure 5.4: The ODF obtained from the optimal process solution, at 20% plastic strain (Example 14).

Figure 5.5: Variation of the objective function with optimization iterations (Example 14).
It was observed that the optimal solution predicted was as accurate as the solution predicted in Section 5.4.3. Numerous design examples in [59, 58] have also shown that the use of the reduced-order approach helps reduce the number of controlled parameters and hence improve the efficiency of the design simulator. In the same breath, it was observed that certain design problems [59] under-performed with the use of reduced-order models. In these cases, it was observed that multiple process solutions resulted in the same objective. This is attributed to the lack of sufficient process information in the reduced-order models. This issue of sufficiency and completeness (i.e. how many POD modes and which modes to use) is an open issue and warrants focused attention in the future.
5.4.5 Example 16: Lagrangian analysis - two-stage process design (at a material point) for desired ODF

In the design for complex microstructures, it is highly unlikely that a single stage would result in the desired microstructure. These problems need to be readdressed in the context of multi-stage design - an attempt to address multi-stage design for isotropic materials was conducted in Section 3.6.4. As developed in Section 3.6.4, multi-stage design (in the context of multi-length scale analysis) is based on a priori selection of a sequence of stages and designing for process parameters in each of these stages. This example motivates the effectiveness of such a scheme for polycrystalline materials, through a design at a material point.

Consider a two-stage process where in the second stage is predefined. The parametrization of the velocity gradient, defined in Equation (5.41), is utilized to define the process. The velocity gradient in the second stage (stage 2), is then
defined a priori, as:

\[ \beta_{\text{stage}2} = \{0, 1, 0, 0, 0, 0, 0, 0\} \quad (5.46) \]

The problem of interest is to design the preforming stage (first stage), i.e., identify the velocity gradient in stage 1, so as to obtain a desired texture at the end of the process (stage 1 followed by stage 2). In addition, the initial texture, i.e. the texture prior to the start of stage 1, is assumed to be random. The objective function is then defined as:

\[ \min_{\beta_{\text{stage}1}} F(\beta) = \frac{1}{N_s} \sum_{i=1}^{N_s} (A_i(\beta) - A_i^{\text{desired}})^2 \quad (5.47) \]

where \(A^{\text{desired}}\) is the desired ODF at the end of the process and is shown in Figure 5.8.

The initial guess to the design problem was assumed as the zero velocity gradient,

\[ \beta_{\text{stage}1\text{guess}} = \{0, 0, 0, 0, 0, 0, 0\} \quad (5.48) \]

The steepest descent optimization scheme was utilized and the variation of the objective function with iteration index is shown in Figure 5.9. The ODF obtained

Figure 5.8: The desired ODF in the multi-stage optimization problem at a material point (Example 16).
Figure 5.9: Variation of the objective function with optimization iterations (Example 16).

through the optimal process solution is shown in Figure 5.10. The converged (optimal) velocity gradient, for stage 1, was computed as:

$$\beta_{optimal} = \{0.504, -0.005, 5E-04, 0.04, -0.007, 1E-04, 2E-04, -3E-04\} \quad (5.49)$$

while the global solution was observed at:

$$\beta_{global-solution} = \{0.50, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0\} \quad (5.50)$$
Chapter 6

Suggestions for future research

The current research effort has tried to develop a framework, for the design of metal forming processes, that can accurately model the thermo-mechanical processing of a wide range of materials. It has also developed a framework for the multi-length scale design of polycrystalline materials and has addressed several issues ranging from the definition of sensitivities of ODF’s to reduced-order modeling of the evolution of texture. In addition, a wide variety of problems were addressed through the developed formulation. Although these examples tried to mimic particular industrial situations, several new developments can broaden its applicability and scope. Suggestions for the continuation of this study on the design optimization of metal forming processes are provided next.

6.1 Direct deformation problem

1. Modeling of multiple deformable (elastic/elasto-plastic) dies which requires the development of algorithms for multi-body deformations (a single rigid die is used in this work). Models that represent thermo-mechanical contact (which
take into account the effect of temperature on normal and tangential contact and the effect of contact pressure of the heat transfer across the die-workpiece interface) need to be incorporated in the analysis.

2. Extend the formulation to address 3–D geometries. Adaptive remeshing that allows for mesh-size gradients in the workpiece must be used in order to accurately represent metal deformation in thin-sections and near regions where the die has a high curvature. The adaptive mesh generation process can be driven by finite element error indicators as well as the geometric features of the specific process being analyzed.

3. Extending the multi-length scale analysis towards macro analysis. Models that represent twinning behavior of metals needs to be incorporated [76]. New algorithms need to be developed to study the feasibility of developing reduced-order models for texture evolution through a Lagrangian analysis.

6.2 Sensitivity deformation problem

A comprehensive computational framework for the shape and parameter sensitivity analysis of metal forming processes has been derived in this work that will provide a strong foundation for further developments such as:

1. Development of a composite error indicator using error estimates from both the direct as well as the sensitivity analysis for the purpose of an adaptive mesh analysis suitable for complex forming design optimization applications.

2. Extending the developed multi-length scale analysis towards h.c.p materials. In particular, sensitivity analysis in the context of microstructure undergoing
twinning is an open issue.

### 6.3 Issues in metal forming design

Eventhough the developed design methodology has proved very accurate, standard industrial problems involve more features in thermo-mechanical processes. They include multiple dies, deformation in thin sections, self-contact to model folding defects and texture evolution at the macroscopic level. Some of the design issues that can be addressed, as an extension of the developments in the thesis, include:

1. Exploiting the synergy between process sequence selection and texture classification. The reduced-order models, POD modes are useful information that can be used towards this end.

2. Extending process design to classification of microstructures.

3. The performance of heuristic optimization schemes, like the response surface technique [77], need to be studied. Such techniques can help find a quicker approximation of the global solution and also provide reliability information for the designed solution.

4. Uncertainty in process and material parameters needs to be incorporated into the design simulator in order to be able to design processes that are robust.
Appendix A

Material properties

A.1 2024 – T351 Aluminum alloy

The flow function \( f (\sigma_m, s, \theta) \) is given as

\[
f (\sigma_m, s, \theta) = \dot{\varepsilon}_p = \dot{\varepsilon}_o \exp \left[ \frac{1}{C} \left( \frac{\sigma_m}{s \left( \frac{\theta_m - \theta_o}{\theta_m - \theta_o} \right) \alpha} - 1 \right) \right]
\]  
(A.1)

and the state variable \( s \) is given explicitly as

\[
s(t) = A + B \ (e^p)^n
\]  
(A.2)

where the equivalent plastic strain \( e^p \) is defined as

\[
e^p = \int_0^t f (\sigma_m, s, \theta) \ dt
\]  
(A.3)

The specific values of the mechanical and thermal parameters are given in Table A.1 and are taken from [78]. The elastic properties are taken as follows:

\[
\mu_m = \mu_{m,o} \left( 1 - \xi_1 \frac{\theta - \theta_o}{\theta_m} \right)
\]  
(A.4)

\[
\kappa_m = \kappa_{m,o} \left( 1 - \xi_2 \frac{\theta - \theta_o}{\theta_m} \right)
\]  
(A.5)

\[
\]  
(A.6)
Table A.1: Material parameters for 2024 – T351 Al at an initial temperature of 300K.

<table>
<thead>
<tr>
<th>Material Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>263.28 MPa</td>
</tr>
<tr>
<td>$B$</td>
<td>421.72 MPa</td>
</tr>
<tr>
<td>$C$</td>
<td>0.015</td>
</tr>
<tr>
<td>$\dot{\epsilon}_0$</td>
<td>0.577 sec$^{-1}$</td>
</tr>
<tr>
<td>$\theta_o$</td>
<td>300 K</td>
</tr>
<tr>
<td>$\theta_m$</td>
<td>775 K</td>
</tr>
<tr>
<td>$\xi_1$</td>
<td>0.5</td>
</tr>
<tr>
<td>$\xi_2$</td>
<td>0.333</td>
</tr>
<tr>
<td>$a$</td>
<td>2</td>
</tr>
<tr>
<td>$n$</td>
<td>0.34</td>
</tr>
<tr>
<td>$\mu_{m,o}$</td>
<td>26 GPa</td>
</tr>
<tr>
<td>$\kappa_{m,o}$</td>
<td>68 GPa</td>
</tr>
<tr>
<td>$\beta_m$</td>
<td>$22.6 \times 10^{-6}$/ K</td>
</tr>
<tr>
<td>$K$</td>
<td>160.0 N/(secs-K)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>2770 Kg/m$^3$</td>
</tr>
<tr>
<td>$c$</td>
<td>875 J/(Kg-K)</td>
</tr>
<tr>
<td>$\omega$</td>
<td>0.90</td>
</tr>
</tbody>
</table>
Here, the subscript $m$ refers to the properties of the matrix material and the subscript $o$ refers to properties specified at the reference temperature $\theta_o$ [78]. The method described by Budiansky [79] was used to calculate the elastic properties $\mu = \mu(\theta, f)$ and $\kappa = \kappa(\theta, f)$ of the porous material (composite) in terms of the elastic properties of the matrix material. This process is summarized below:

$$\sum_{i=1}^{N} f_i \left[ 1 - a + a \left( \frac{\kappa_i}{\kappa} \right) \right]^{-1} = 1$$  \hspace{1cm} (A.7)

$$\sum_{i=1}^{N} f_i \left[ 1 - b + b \left( \frac{\mu_i}{\mu} \right) \right]^{-1} = 1$$  \hspace{1cm} (A.8)

where the subscript $i$ denotes the properties of the $i^{th}$ material and $\kappa$ and $\mu$ are the elastic properties of the composite. Also,

$$a = \frac{1}{3} \left\{ \frac{1 + \nu}{1 - \nu} \right\}$$  \hspace{1cm} (A.9)

$$b = \frac{2}{15} \left\{ \frac{4 - 5\nu}{1 - \nu} \right\}$$  \hspace{1cm} (A.10)

and $\nu$, the Poisson’s ratio of the composite is given as

$$\nu = \frac{3\kappa - 2\mu}{6\kappa + 2\mu}$$  \hspace{1cm} (A.11)

### A.2 0.2% C Steel (Cast)

The evolution of the equivalent plastic strain (Equation (2.20)) is defined as follows:

$$f(\sigma_m, s, \theta) = \dot{\varepsilon}^p = \dot{\varepsilon}_0 \exp \left( \frac{-Q}{R\theta} \right) \left( \frac{L_0}{L} \right)^w \left[ \sinh \left( \frac{\sigma_m}{\zeta s} \right) \right]^{1/n_1}$$  \hspace{1cm} (A.12)

where the material parameters are defined in Table A.2. The evolution of the deformation resistance, i.e., the hardening law is defined by the following equation:

$$h(\sigma_m, s, \theta, L) = h_s \left[ 1 - \frac{s}{s^*} \right]^a \text{sign} \left( 1 - \frac{s}{s^*} \right) \dot{\varepsilon}^p$$  \hspace{1cm} (A.13)
where \( s^* \), the dynamically stable value of \( s \), is defined as

\[
s^* = \chi \left\{ \frac{\dot{e}^p}{\dot{e}_0} \exp \left( \frac{Q}{R\theta} \right) \left( \frac{L^*}{L_0} \right)^w \right\}^{n_2} \tag{A.14}
\]

where \( \chi \) and \( n_2 \) are material parameters. The kinetics of grain growth are defined through the evolution of the mean grain size as:

\[
\dot{L} = - f_R X_R \dot{L} - L^* \dot{\epsilon}^p + \dot{L}_0 (1 - \exp(-X_R - X_{Rc} \dot{\epsilon}^p)) \exp \left( - \frac{Q}{R\theta} \right) \left( \frac{L_o}{L} \right) \tag{A.15}
\]

where \( f_R, \dot{L}_0 \) are material constants, \( X_R \) denotes the volume fraction of grains recrystallized and \( X_{Rc} \) is the volume fraction recrystallized at the end of primary recrystallization. The volume fraction of grains recrystallized is given through the following expression [4]:

\[
X_R = 1 - \exp \left\{ - f_X \frac{L_o}{L^*} \left( \frac{\tilde{\epsilon}^p - \tilde{\epsilon}^p_C}{\tilde{\epsilon}^p} \right) \right\} \tag{A.16}
\]

Furthermore, the critical strain for the onset of recrystallization is given by:

\[
\tilde{\epsilon}^p_C = \frac{2}{\sqrt{3}} \frac{C_c}{\mu} (f_C S^* - S_0) \tag{A.17}
\]

where \( C_c, f_C \) are prescribed material parameters and \( \tilde{\epsilon}^p_R \), the strain at the end of primary recrystallization, is given by [4]

\[
\tilde{\epsilon}^p_R = \frac{2}{\sqrt{3}} \frac{C_R}{\mu} s_0 f_1 (L, L^*) \tag{A.18}
\]

where \( C_c, C_R, f_C \) are material parameters and \( f_1 \) is a function measuring the dynamic imbalance. Additionally, an implicit relation [4] for the dynamically stable recrystallized mean grain size in terms of the strain rate, the absolute temperature and the initial grain size is given as follows:

\[
L^* = \left( \frac{q}{\zeta \chi A^{n_2}} \right)^{1/p} \left\{ \ln(A^{n_1} + \sqrt{A^{2n_1} + 1}) \right\}^{-1/p} \tag{A.19}
\]

\[
A = \frac{\dot{\epsilon}^p L^* w}{\dot{e}_0 L_o} \exp \left( \frac{Q}{R\theta} \right) \tag{A.20}
\]
A Newton type iterative procedure is used to evaluate $L^*$ given the values of $\dot{\varepsilon}^p, \theta$ and $L_o$.

A.3 Fe - 2.0% Si

The constitutive model used is defined as follows:

$$f(\sigma_m, s, \theta) = \dot{\varepsilon}^p = A \exp\left(-\frac{Q}{R\theta}\right) \left[\sinh(\xi\sigma_m/s)\right]^{1/m}$$  \hspace{1cm} (A.21)

$$h(\sigma_m, s, \theta) = h_0 \left|1 - \frac{s}{s^*}\right|^a$$  \hspace{1cm} (A.22)

where

$$s^* = \tilde{s} \left[f(\sigma_m, s, \theta)/A \exp\left(\frac{Q}{R\theta}\right)\right]^n$$  \hspace{1cm} (A.23)

The specific values of the mechanical and thermal parameters are given in Table A.3.

A.4 Simple power law model

The functional form for the strain rate, using a power law model, with material rate sensitivity $m$, and the matrix material is assumed not to harden [80]

$$f(\sigma_m, s) = \dot{\varepsilon}^p = \dot{\varepsilon}_0 \left\{\frac{\sigma_m}{s}\right\}^{1/m}$$  \hspace{1cm} (A.24)

where $\dot{\varepsilon}_0 = 10^{-03}$ sec$^{-1}$, $m = 0.05$ and $s = 150$ MPa.

A.5 F.C.C 99.987% Aluminum

The anisotropic elasticity tensor for f.c.c aluminum can be specified in terms of the three stiffness parameters (crystal stiffness tensor $C$ in the crystal frame) which are
approximated (in GPa) in terms of the temperature \( \theta \) (in K) as follows [8]

\[
\begin{align*}
c_{11} &= 123.323 + 6.7008 \times 10^{-8} \theta^3 - 1.1342 \times 10^{-4} \theta^2 - 7.8788 \times 10^{-3} \theta \\
c_{12} &= 70.6512 + 4.4105 \times 10^{-8} \theta^3 - 7.5498 \times 10^{-5} \theta^2 + 3.9992 \times 10^{-3} \theta \\
c_{44} &= 31.2071 + 7.0477 \times 10^{-9} \theta^3 - 1.2136 \times 10^{-5} \theta^2 - 8.3274 \times 10^{-3} \theta
\end{align*}
\] (A.25)

Furthermore, the saturation values of the slip system resistances were taken equal for all slip systems and were evaluated from [75] as

\[
\begin{align*}
s_s(20K) &= 214 \text{ MPa}; \\
s_s(140K) &= 88.0 \text{ MPa}; \\
s_s(195K) &= 70.0 \text{ MPa}; \\
s_s(300K) &= 50.6 \text{ MPa}.
\end{align*}
\]

Additional material properties are listed in Table A.4. An isotropic thermal expansion coefficient is taken equal to \( 2.3E - 05K^{-1} \).

### A.6 1100–Aluminum alloy

The specific constitutive model used is defined as follows (refer to Equations (2.20) and (2.21)) [80, 81]:

\[
\begin{align*}
f(\sigma_m, s, \theta) &= \dot{\varepsilon}^p = A \exp\left(-\frac{Q}{R\theta}\right) \left[\sinh\left(\xi \frac{\sigma_m}{s}\right)\right]^{1/m} \\
h(\sigma_m, s, \theta) &= h_0 \left[1 - \frac{s}{s^*}\right]^{a}
\end{align*}
\] (A.26, A.27)

where

\[
s^* = \tilde{s} \left[\frac{f(\sigma_m, s, \theta)}{A} \exp\left(\frac{Q}{R\theta}\right)\right]^n
\] (A.28)

The specific values of the mechanical and thermal parameters are given in Table A.5.
Table A.2: Material parameters for 0.2% C steel at 1213K.

<table>
<thead>
<tr>
<th>Material Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{\varepsilon}_0 )</td>
<td>( 2.618 \times 10^{11} \text{ sec}^{-1} )</td>
</tr>
<tr>
<td>( Q )</td>
<td>283 KJmol(^{-1})</td>
</tr>
<tr>
<td>( \mu )</td>
<td>57.69 GPa</td>
</tr>
<tr>
<td>( \kappa )</td>
<td>125.0 GPa</td>
</tr>
<tr>
<td>( K )</td>
<td>32.5 ( \text{N/(sec-K)} )</td>
</tr>
<tr>
<td>( \rho_c )</td>
<td>4.884 MN/(m(^2)-K)</td>
</tr>
<tr>
<td>( \omega )</td>
<td>0.90</td>
</tr>
<tr>
<td>( L_o )</td>
<td>91.0 Microns</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>0.308</td>
</tr>
<tr>
<td>( n_1 )</td>
<td>0.11</td>
</tr>
<tr>
<td>( s_0 )</td>
<td>150.0 MPa</td>
</tr>
<tr>
<td>( \chi )</td>
<td>431 Mpa</td>
</tr>
<tr>
<td>( h_s )</td>
<td>7800</td>
</tr>
<tr>
<td>( a_s )</td>
<td>1.55</td>
</tr>
<tr>
<td>( n_2 )</td>
<td>0.069</td>
</tr>
<tr>
<td>( f_R )</td>
<td>120</td>
</tr>
<tr>
<td>( f_C )</td>
<td>0.728</td>
</tr>
<tr>
<td>( C_C )</td>
<td>59</td>
</tr>
<tr>
<td>( p )</td>
<td>0.8</td>
</tr>
<tr>
<td>( q )</td>
<td>5 N mm(^{p-2})</td>
</tr>
<tr>
<td>( f_X )</td>
<td>1.0</td>
</tr>
<tr>
<td>( \dot{L}_0 )</td>
<td>( 6.0 \times 10^6 \text{ m sec}^{-1} )</td>
</tr>
</tbody>
</table>
Table A.3: Material parameters for Fe-2% Si at a temperature of 1273K.

<table>
<thead>
<tr>
<th>Material Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$6.346 \times 10^{11}$ sec$^{-1}$</td>
</tr>
<tr>
<td>$Q/R$</td>
<td>$3.756916 \times 10^{4}$ K$^{-1}$</td>
</tr>
<tr>
<td>$\xi$</td>
<td>3.25</td>
</tr>
<tr>
<td>$m$</td>
<td>0.1956</td>
</tr>
<tr>
<td>$s_0$</td>
<td>66.1 MPa</td>
</tr>
<tr>
<td>$h_0$</td>
<td>3093.1 MPa</td>
</tr>
<tr>
<td>$a$</td>
<td>1.5</td>
</tr>
<tr>
<td>$\dot{s}$</td>
<td>125.1 MPa</td>
</tr>
<tr>
<td>$n$</td>
<td>0.06869</td>
</tr>
<tr>
<td>$\mu$</td>
<td>37.23 GPa</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>194.45 GPa</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$11.80 \times 10^{-6}$/ K</td>
</tr>
<tr>
<td>$K$</td>
<td>80.0 N/(secs-K)</td>
</tr>
<tr>
<td>$\rho c$</td>
<td>$2.47 \times 10^6$ J/(m$^3$-K)</td>
</tr>
<tr>
<td>$\omega$</td>
<td>0.90</td>
</tr>
</tbody>
</table>
### Table A.4: Material properties of f.c.c Aluminum.

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{\gamma}^0$</td>
<td>1.732E+06 /s</td>
</tr>
<tr>
<td>$h_0$</td>
<td>250 MPa</td>
</tr>
<tr>
<td>$r_1$</td>
<td>2.0</td>
</tr>
<tr>
<td>$p$</td>
<td>0.141</td>
</tr>
<tr>
<td>$q$</td>
<td>1.1</td>
</tr>
<tr>
<td>$s_{at,0}$</td>
<td>8.76 MPa</td>
</tr>
<tr>
<td>$s_{t,0}$</td>
<td>8.76 MPa</td>
</tr>
<tr>
<td>$\eta$</td>
<td>1.0</td>
</tr>
<tr>
<td>$\rho$</td>
<td>2.77 Mg/m$^3$</td>
</tr>
<tr>
<td>$c$</td>
<td>920.0 J/kg-K</td>
</tr>
</tbody>
</table>
Table A.5: Material properties of 1100-Aluminum at 673K.

<table>
<thead>
<tr>
<th>Material Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$1.90593 \times 10^7$ sec$^{-1}$</td>
</tr>
<tr>
<td>$Q/R$</td>
<td>$2.1086 \times 10^4$ K$^{-1}$</td>
</tr>
<tr>
<td>$\xi$</td>
<td>7.0</td>
</tr>
<tr>
<td>$m$</td>
<td>0.23348</td>
</tr>
<tr>
<td>$s_0$</td>
<td>29.7 MPa</td>
</tr>
<tr>
<td>$h_0$</td>
<td>1115.6 MPa</td>
</tr>
<tr>
<td>$a$</td>
<td>1.3</td>
</tr>
<tr>
<td>$\dot{s}$</td>
<td>18.92 MPa</td>
</tr>
<tr>
<td>$n$</td>
<td>0.07049</td>
</tr>
<tr>
<td>$\mu$</td>
<td>20.2 GPa</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>66.0 GPa</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$26.5 \times 10^{-6}$ K$^{-1}$</td>
</tr>
<tr>
<td>$K$</td>
<td>238.0 N/(sec-K)</td>
</tr>
<tr>
<td>$\rho c$</td>
<td>2.820 MN/(m$^2$-K)</td>
</tr>
<tr>
<td>$\omega$</td>
<td>0.90</td>
</tr>
</tbody>
</table>
Appendix B

Time integration algorithms

B.1 Time integration of $\mathring{\mathbf{R}}^e$

The evolution equation for $\mathring{\mathbf{R}}^e$ is given as: (Equation (5.22))

$$\mathring{\Omega} = \mathring{\mathbf{R}}^e \mathring{\mathbf{R}}^e T - \Omega \mathring{\mathbf{R}}^e \mathbf{R}^e T$$ \hspace{1cm} (B.1)

where $\mathring{\mathbf{R}}^e T = - \mathbf{R}^e T \mathring{\mathbf{R}}^e \mathbf{R}^e T$. Consider the following:

$$\frac{\partial}{\partial t} \left[ \mathring{\mathbf{R}}^e \mathbf{R}^e T \right] = \mathring{\mathbf{R}}^e \mathbf{R}^e T - \mathbf{R}^e \mathbf{R}^e T \mathring{\mathbf{R}}^e \mathbf{R}^e T$$

$$= \mathring{\mathbf{R}}^e \mathbf{R}^e T - \mathbf{R}^e \mathbf{R}^e T \mathring{\mathbf{R}}^e \mathbf{R}^e T$$ \hspace{1cm} (B.2)

where $\Omega = \mathring{\mathbf{R}}^e \mathbf{R}^e T$.

Using Equations (B.1) and (B.2), we obtain

$$\frac{\partial}{\partial t} \left[ \mathring{\mathbf{R}}^e \mathbf{R}^e T \right] - \mathring{\mathbf{R}}^e \mathbf{R}^e T + \mathbf{R}^e \mathbf{R}^e T \Omega = \mathring{\Omega}$$ \hspace{1cm} (B.3)

Employing the Euler backward integration scheme, over $(t_n, t_{n+1})$, to integrate Equation (B.3) results in:

$$\frac{\partial}{\partial t} \left[ \mathring{\mathbf{R}}^e \mathbf{R}^e T \right] - \Omega_{n+1} \mathring{\mathbf{R}}^e \mathbf{R}^e T + \mathbf{R}^e \mathbf{R}^e T \Omega_{n+1} = \mathring{\Omega}$$ \hspace{1cm} (B.4)
Premultiplying by \( \exp(-t\Omega_{n+1}) \), postmultiplying by \( \exp(t\Omega_{n+1}) \) and integrating, we obtain:

\[
R_e^{n+1} R_e^{T n+1} = \Delta R_e^{n+1} R_e^{n} R_e^{T n} (\Delta R_e)^T_{n+1} + \Delta t \Omega_{n+1}
\]  

(B.5)

where, from the direct problem,

\[
\Delta R_e^{n+1} = R_e^{n+1} R_e^{T n} = \exp(\Delta t \Omega_{n+1})
\]  

(B.6)

and \( \Delta t = t_{n+1} - t_n \). Equation (B.5) can be re-arranged to obtain the following:

\[
\Omega = \frac{1}{\Delta t} \left[ R_e R_e^{T} - R_e^{T n} R_e^{T n} R_e R_e^{T} \right]
\]  

(B.7)

where the subscript \((n+1)\) has been dropped for convenience.

**B.2 Time integration of \( \overset{\circ}{r} \)**

The evolution equation for the sensitivity of the re-orientation is given by (Equation (5.24))

\[
\frac{\partial \overset{\circ}{r}}{\partial t} - M_2 \overset{\circ}{r} = \frac{1}{2} \left( \overset{\circ}{\omega} + (\overset{\circ}{\omega} \cdot \overset{\circ}{r}) \overset{\circ}{r} + \overset{\circ}{\omega} \times \overset{\circ}{r} \right)
\]  

(B.8)

where \( M_2 = \frac{1}{2} \{ \omega \otimes r + (\omega \cdot r)I + \Omega \} \). Similar to the analysis performed in Appendix B.1, employ the Euler backward integration scheme to integrate Equation (B.8) and re-write the equation as:

\[
\frac{\partial \overset{\circ}{r}}{\partial t} - M_{2, n+1} \overset{\circ}{r} = \frac{1}{2} \left( \overset{\circ}{\omega}_{n+1} + (\overset{\circ}{\omega}_{n+1} \cdot r_{n+1}) r_{n+1} + \overset{\circ}{\omega}_{n+1} \times r_{n+1} \right)
\]  

(B.9)

Premultiplying by \( \exp(-tM_{2, n+1}) \) and integrating, we obtain:

\[
\overset{\circ}{r}_{n+1} = \exp(\Delta t M_{2, n+1}) \overset{\circ}{r}_n + \\
\frac{\Delta t}{2} \left[ \overset{\circ}{\omega}_{n+1} + (\overset{\circ}{\omega}_{n+1} \cdot r_{n+1}) r_{n+1} + \overset{\circ}{\omega}_{n+1} \times r_{n+1} \right]
\]  

(B.10)

which can be re-written in the form of Equation (4.42).
Appendix C

Additional implementation details

C.1 Bézier curve: Bernstein functions

A degree $n$ Bézier curve can be defined using $i = 1, \cdots, (n + 1)$ basis functions as

$$f^n_B(\alpha) = \sum_{i=1}^{n+1} \beta_i f_i(\alpha) \quad (C.1)$$

where the Bernstein functions $f_i(\alpha)$ are given as

$$f_i(\alpha) = \frac{n!}{(i-1)!(n-i+1)!} \alpha^{i-1} (1 - \alpha)^{n-i+1} \quad (C.2)$$

with $\alpha \in [0, 1]$ and $\beta_i, i = 1, \cdots, (n + 1)$ being algebraic control parameters.

C.2 Extending the object oriented framework for metal forming design

An object oriented (OO) programming framework was developed in [1] and has been extended, here, towards the development of a realistic design simulator. The class structure developed in this framework is generic and hence is easily extendable. This
Figure C.1: A schematic of the object oriented framework for the developed sensitivity analysis.

development utilizes the object oriented development of \texttt{Diffpack}. The framework of the developed simulator is shown in Figure C.1. A list of some of the abstract data types developed as part of the design simulator is shown below.

1. **Thermo-mechanical problem:**

\texttt{ThermalLargeDef} (Coupled thermal and deformation analysis)

    - **Mechanical problem:**
        - \texttt{LargeDef} (Large deformation FE analysis)
        - Forging, Extrusion, Drawing, TensionTest

    - **Constitutive problem:**
ConstitutiveBase (Material properties)
ConstitutiveIntegration (Time integration schemes)
    IsotropicRateDependent, PolycrystalRateDependentModel

Orientation distribution function (ODF) problem:
ODFIntegration (Lagrangian; Eulerian - full model, reduced-order model)

Kinematic problem:
Deformation (Deformation gradient related computations)

Thermal problem:
NonLinearHeat (Non linear FE conduction analysis)
    HeatForging, HeatExtrusion

2. Sensitivity thermo-mechanical problem:
    SensitivityLargeDef (Parameter sensitivity FEA)
        ShapeSensitivity (Shape sensitivity FEA)
            SensitivityLargeDefUL (Updated Lagrangian parameter sensitivity)
            ShapeSensitivityUL (Updated Lagrangian shape sensitivity)

Sensitivity constitutive problem:
SensitivityConstitutive
    SensitivityRateDependent, SensitivityPolycrystalRateDependent

Sensitivity thermal problem:
    SensitivityNonLinearHeat (Linear sensitivity thermal analysis)
        SensitivityHeatForging, SensitivityHeatExtrusion

Sensitivity ODF problem:
SensitivityODF (Sensitivity of ODF, fundamental regions)

3. Optimization problem:
ObjectivesAndConstraint (User defined optimization problem features)
OptimizationMethod (Steepest descent, BFGS)

4. Multi-stage problems:

TwoStageProcess (Two stage forming sequence analysis)

TwoStageSensitivity (Two stage forming sequence sensitivity analysis)

TwoStageOptimization (Two stage forming sequence design)
Bibliography


