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**Computational and Applied Mathematics**

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**Hybrid Modeling of Porous Metal Plasticity:  
Integrating Micromorphic Theories with  
Data-Driven Methods.**

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## Abstract

This study presents a hybrid analytical and data-driven framework for modeling micromorphic porous plastic materials subjected to complex loading. Using the Gologanu-Leblond-Perrin-Devaux (GLPD) model, we integrate higher-order stress gradients and microstructural effects into the analysis of a hollow sphere under hydrostatic tension. The research extends the theory of classical porous plasticity by incorporating microstructural length scales, enabling a more accurate description of the growth of gaps and the localization of damage. Analytical solutions are derived and benchmarked against classical von Mises plasticity in the limit of vanishing nonlocal effects. Stability and bifurcation analysis reveals critical thresholds for material failure, while a dimensionless formulation highlights key governing parameters. Additionally, we employ machine learning techniques, specifically Gaussian Process Regression, to develop a surrogate model for predicting bifurcation points, demonstrating the potential of data-driven approaches in enhancing computational efficiency. This work bridges theoretical modeling and experimental validation, offering a robust framework for understanding and predicting the behavior of advanced porous materials in engineering applications.

*Keywords:* Micromorphic model, Machine Learning, Bifurcation Analysis, Metal Plasticity, Data-driven Analysis

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## 1. Introduction

Ductile fracture in porous plastic materials remains a significant challenge in mechanical and materials science. Traditional models such as the Gurson-Tvergaard-Needleman (GTN) framework [14, 24] have been extensively used to describe void growth and coalescence in metal plasticity. However, these models often fail to capture nonlocal effects arising from microscale interactions. Several studies have attempted to introduce gradient-based theories to improve accuracy [9, 1, 2]. Recent research in micromorphic theories [10, 12] has demonstrated the benefits of incorporating higher-order stress gradients to account for size effects and strain localization. Inclusion of microstructural length scales in constitutive models has been shown to provide better predictions of material behavior in dynamic loading scenarios. Additionally, advancements in machine learning techniques have enabled the development of surrogate models that capture complex mechanical behavior more efficiently [4, 13]. These data-driven approaches complement traditional methods by providing real-time predictions and enabling uncertainty quantification [22].

The challenge of accurately modeling ductile fracture is crucial for applications in aerospace, automotive, and biomedical engineering, where material failure can lead to catastrophic consequences. Standard plasticity models assume uniform deformation fields, neglecting microscale heterogeneities that influence void growth and damage localization. The incorporation of micromorphic effects provides a more refined description of stress and strain evolution, improving the predictive capabilities of constitutive models [8]. Second-gradient theories [11, 19] introduce characteristic length scales that enable models to capture the physics of material deformation more accurately, leading to improved failure predictions.

The Gologanu-Leblond-Perrin-Devaux (GLPD) model [12] extends classical porous plasticity models by integrating microstructural considerations into the constitutive equations. This study focuses on a specific problem: the response of a hollow sphere made of micromorphic porous plastic material subjected to hydrostatic tension. We derive analytical solutions and compare them to classical models such as von Mises plasticity in the limit of vanishing length-scale effects [20, 15]. Previous work by Gologanu et al. [12] introduced the concept of higher-order stress tensors in porous media, which provided insights into deformation mechanisms. Additionally, the work by Needleman and Tvergaard [21] examined numerical simulations of porous materials, highlighting discrepancies between classical and nonlocal approaches. Machine learning models, such as physics-informed neural networks (PINNs) [22], have been increasingly applied to solve partial differential equations governing micromorphic models, offering a novel perspective on data-driven mechanics [16].

Existing numerical studies [27] have confirmed that micromorphic models significantly enhance failure predictions compared to classical theories. These models account for microstructural effects in materials, making them more capable of capturing the complexities of failure mechanisms such as strain localization and ductile rupture. Additional studies by Enakoutsa et al. [5] implemented micromorphic models in numerical simulations and achieved mesh-independent results, accurately reproducing experimental observations. Similarly, Ulloa et al. [25] developed a data-driven micromorphic framework for materials with strain localization, demonstrating the potential for enhanced computational

efficiency and predictive capabilities in plasticity models.

The integration of machine learning techniques has further strengthened the ability to model complex material behavior, particularly through surrogate modeling approaches such as Gaussian process regression [23]. These methods significantly reduce computational costs while maintaining high accuracy [17, 26]. However, while previous work has established the theoretical foundations for higher-order stress contributions [12], analytical solutions remain scarce due to the complexity of governing equations.

This paper addresses this gap by deriving explicit solutions for a hollow-sphere problem, providing insights into the role of microstructural length scales in ductile failure mechanisms. Studies by Besson [3] have focused on numerical strategies for implementing these theories efficiently, while recent advancements in computational mechanics [7] have enabled more precise validation of micromorphic theories against experimental data. Moreover, the integration of data-driven approaches into micromorphic models has introduced novel methodologies for real-time predictions of material behavior [17, 26].

This paper is structured as follows. Section 2 presents the development of the analytic solution and examines the asymptotic behavior of the governing equations, laying the foundation for subsequent theoretical analysis. Section 3 introduces the dimensional analysis of the governing equations, identifying key nondimensional parameters that characterize the system's response and control microstructural effects. Section 4 conducts a stability and bifurcation analysis of the governing ordinary differential equation (ODE), identifying fixed points and assessing their stability to predict material failure mechanisms. Section 5 explores analytical approximation methods, including perturbation analysis and asymptotic expansions, which provide tractable solutions and deeper insight into the behavior of the system under different conditions. Section 6 extends the bifurcation analysis by incorporating micromorphic contributions, thereby bridging the gap between classical and enriched porous plasticity theories. Section 7 introduces a surrogate modeling framework based on Gaussian Process Regression (GPR) to efficiently predict bifurcation points, reducing computational costs while maintaining accuracy. Finally, Section 8 presents our concluding remarks, summarizing the key findings, discussing their broader implications in micromechanics and computational plasticity, and outlining future research directions, including possible extensions to multiscale modeling and machine learning-enhanced simulations.



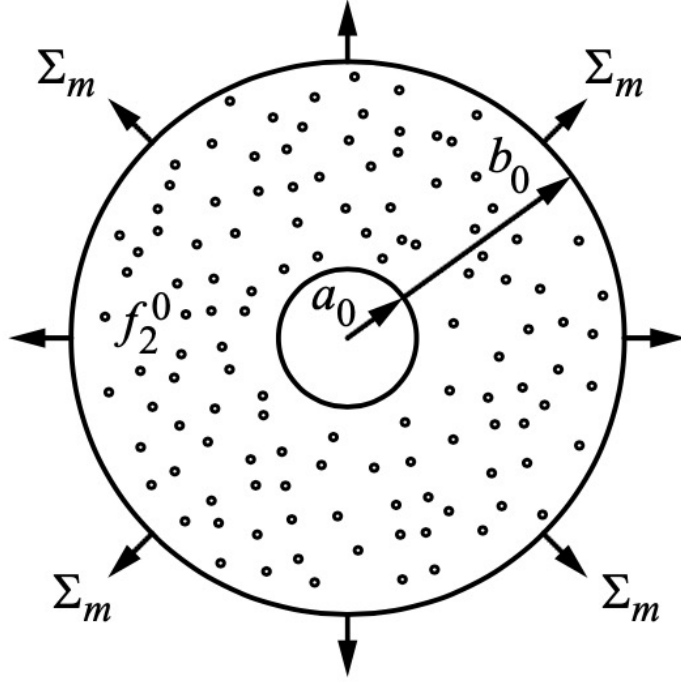


Figure 1: The hollow sphere model problem being considered.

## 2. The hollow porous sphere problem

We consider a hollow sphere with inner radius  $a_0$  and outer radius  $b_0$ , representing an elementary cell of a porous plastic metal; see Figure 1. The matrix contains small secondary dispersed voids; its porosity (void volume fraction) is initially uniform and is denoted  $f_0^2$ . The boundary of the central void is free from traction, whereas the outer boundary is subjected to some general hydrostatic tension  $\Sigma_m$ . The matrix material of the porous hollow sphere is supposed to obey the GLPD constitutive model as described in Appendix B and in [12]. The hollow sphere model problem presented here has served to find the solutions of several ductile fracture problems the solution of which has yielded micromechanics-based models for ductile porous metals under various loading conditions.

### 2.1. Analytical solution when porosity is neglected

#### 2.1.1. Derivation of the mechanical fields

We seek a solution to the problem of the spherical shell for the behavior of purely ideal plastic, the stress of the yield in simple tension being denoted by  $\Sigma_0$  and the porosity in the matrix being neglected. As a result, the yield criterion of the GLPD model reduces to

$$\Phi(\boldsymbol{\Sigma}, \boldsymbol{M}, \Sigma) \equiv \frac{1}{\Sigma^2} \left( \Sigma_{\text{eq}}^2 + \frac{Q^2}{b^2} \right) - 1 = 0. \quad (1)$$

In this equation:

- $\boldsymbol{\Sigma}$  represents the ordinary second-rank symmetric Cauchy stress tensor and  $\boldsymbol{M}$  is the third-rank moment tensor, symmetric in its first two indices only. The components of  $\boldsymbol{M}$  satisfy

$$M_{ijj} = 0. \quad (2)$$

- $\Sigma_{\text{eq}} \equiv \left(\frac{3}{2}\boldsymbol{\Sigma}' : \boldsymbol{\Sigma}'\right)^{\frac{1}{2}}$  is the von Mises equivalent stress,  $\boldsymbol{\Sigma}'$  being the deviator of  $\boldsymbol{\Sigma}$ .
- $\Sigma$  represents a kind of average yield stress in the heterogeneous metallic matrix.
- $Q^2$  is a quadratic form of the components of the moment tensor given by

$$\begin{aligned} Q^2 &\equiv A_1 \mathcal{M}_1 + A_2 \mathcal{M}_2, \\ A_1 &= 0.194, \quad A_2 = 6.108, \end{aligned} \quad (3)$$

where

$$\begin{aligned} \mathcal{M}_1 &\equiv M_{mk} M_{mk}, \\ \mathcal{M}_2 &\equiv \frac{3}{2} M'_{ijk} M'_{ijk}, \end{aligned} \quad (4)$$

are the quadratic invariants of  $\mathbf{M}$ ; here  $M_{mk} \equiv \frac{1}{3} M_{hhk}$  and  $\mathbf{M}'$  denote the mean and deviatoric parts of  $\mathbf{M}$ , taken over its first two indices.

- $b$  represents the characteristic length scale.

After development, the flow rule becomes (see Gologanu *et al.* [12] for details)

$$\dot{D}_{ij}^p = \eta \frac{3}{\Sigma_0^2} \Sigma'_{ij}, \quad (5)$$

$$(\nabla \dot{D})_{ijk}^p = \frac{\eta}{\Sigma_0^2 b^2} \left( \frac{2}{3} A_1 \delta_{ij} M_{mk} + 3 A_{11} M'_{ijk} \right) + \delta_{ik} U_j + \delta_{jk} U_i. \quad (6)$$

where  $M_{mk} \frac{1}{3} M_{hhk}$  and  $\mathbf{M}'$  are as above and  $\eta$  is the plastic multiplier, determined from the consistency condition and satisfying

$$\eta \begin{cases} = 0 & \text{if } \Phi(\boldsymbol{\Sigma}, \mathbf{M}, \Sigma) < 0, \\ \geq 0 & \text{if } \Phi(\boldsymbol{\Sigma}, \mathbf{M}, \Sigma) = 0. \end{cases} \quad (7)$$

We shall also assume that the parameter  $A_I$  vanishes for the analytical solution to be amenable. Another subtler reason for this choice is that the value of  $A_1$  in the GLPD model, 0.194, is much smaller than that of  $A_{11}$ , 6.108; hence, the value of  $A_1$  can be safely neglected.

We are looking for a solution in which the spherical shell is entirely plastic, so that the yield function  $\Phi(\boldsymbol{\Sigma}, \mathbf{M}, \Sigma_0)$  is zero everywhere. We briefly review the solution procedure given by Burson and Enakoutsa [6]. Consider the velocity, strain rate, and its gradient fields first. As in the case of purely elastic behavior, the matrix of spherical shell is incompressible; as a result, the velocity field is radial and given by

$$\mathcal{U} = \frac{A}{r^2}, \quad (8)$$

where  $A$  is a parameter independent of the material point position  $r$ .

Using the flow rule and the incompressibility of the material, the nonzero components of the stress and moment fields are found to be

$$\Sigma'_{rr} = -\frac{1}{\eta} \frac{2A\Sigma_0^2}{3r^2}, \quad \Sigma'_{\theta\theta} = \Sigma'_{\phi\phi} = \frac{1}{\eta} \frac{A\Sigma_0^2}{3r^2}, \quad (9)$$

$$M'_{rrr} = \frac{1}{\eta} \frac{2A\Sigma_0^2 b^2}{A_{11}r^4}, \quad M_{r\theta\theta} = M_{r\phi\phi} = -\frac{1}{\eta} \frac{A\Sigma_0^2 b^2}{A_{11}r^4}, \quad (10)$$

$$M'_{\theta\theta r} = M'_{\phi\phi r} = -\frac{1}{\eta} \frac{A\Sigma_0^2 b^2}{A_{11}r^4}. \quad (11)$$

The conditions  $M_{ijj} = 0$  and the expressions of  $M'_{rrr}$  and  $M_{r\theta\theta}$  in (8) yield

$$M_{rrr} = -2M_{r\theta\theta}, \quad M_{\theta\theta r} = M'_{\theta\theta r}. \quad (12)$$

Substituting the formulas for stress and moment, in the reduced yield criterion, we get the following expression for the plastic multiplier  $\eta$ :

$$\eta = \frac{A\Sigma_0}{r^3} \sqrt{1 + \frac{15b^2}{A_{11}r^2}}. \quad (13)$$

This completes the specification of the non-zero components of the moment tensor. However, the full expressions of the non-zero components of the ordinary stress tensor are still unknown. After a tedious but straightforward calculation using the expressions of the nonzero components of the moment tensor, the spherical symmetry properties of the problem, and the fact that  $\Sigma_{rr} - \Sigma_{\theta\theta} = \Sigma'_{rr} - \Sigma'_{\theta\theta}$ , the formulas for the nonzero components of the ordinary Cauchy stress tensor are obtained as

$$\frac{d\Sigma_{rr}}{dr} = f(r) \quad (14)$$

with

$$f(r) = \frac{2A\Sigma_0^2}{\eta r^3} + \frac{2(\eta''\eta^2 - 2\eta'^2\eta)}{\eta^4} \frac{A\Sigma_0^2 b^2}{A_{11}r^4} - \frac{28\eta'}{\eta^2} \frac{A\Sigma_0^2 b^2}{A_{11}r^5} - \left( \frac{72}{\eta} + \frac{2\eta'}{\eta^2} \right) \frac{A\Sigma_0^2 b^2}{A_{11}r^6} - \frac{8A\Sigma_0^2 b^2}{\eta A_{11}r^7}, \quad (15)$$

the primes denoting differentiation with respect to  $r$ . Equation (10) implicitly defines the expression of the component  $\Sigma_{rr}$  of the stress tensor. The differentiation of  $\eta$  and some insight into the higher-order differentiation of this plastic multiplier are given in Appendix A and ???. The nonzero components of the stress tensor are obtained as

$$\Sigma_{rr} = \int_{r_i}^r f(\tau) d\tau, \quad \Sigma_{\theta\theta} = \Sigma_{\phi\phi} = \Sigma_{rr} - \frac{1}{\eta} \frac{A\Sigma_0^2}{r^2}. \quad (16)$$

The solution found for the Cauchy stress along with the non-zero components of the moment provided above automatically satisfies the balance equations.

## 2.2. Asymptotic Analysis of the Solution

In this section, we analyze the asymptotic behavior of the solution for the radial stress component, denoted as  $\Sigma_{rr}$ , under the framework of micromorphic plasticity. The governing differential equation governing  $\Sigma_{rr}$  is given by

$$\frac{d\Sigma_{rr}}{dr} = f(r), \quad (17)$$

where the function  $f(r)$  encapsulates the micromorphic contributions and is expressed as

$$f(r) = \frac{2A\sigma_0^2}{r^3} + 2(\eta\eta'' - \eta'^2) \frac{\Sigma_0^2 b^2}{A_{II} r^4} - \frac{(20\eta' + 8\eta\eta')\sigma_0^2 b^2}{A_{II} r^5} - \frac{(72 + 2\eta')\Sigma_0^2 b^2}{A_{II} r^6} - \frac{A\Sigma_0^2 b^2}{A_{II} r^7}. \quad (18)$$

The parameters  $\eta$ ,  $\eta'$ , and  $\eta''$  correspond to the plastic multiplier and its respective derivatives, which are defined as follows:

$$\eta = \frac{A\Sigma_0}{r^3} \sqrt{1 + \frac{15A_{II}b^2}{r^2}}, \quad (19)$$

$$\eta' = -\frac{3A\Sigma_0}{r^4} \sqrt{1 + \frac{15A_{II}b^2}{r^2}} + \frac{15A\Sigma_0 b^2 A_{II}}{r^6 \sqrt{1 + \frac{15A_{II}b^2}{r^2}}}, \quad (20)$$

$$\eta'' = \frac{45A\Sigma_0}{r^5} \sqrt{1 + \frac{15A_{II}b^2}{r^2}} - \frac{135A\Sigma_0 b^2 A_{II}}{r^7 \sqrt{1 + \frac{15A_{II}b^2}{r^2}}} - \frac{225A\Sigma_0 b^4 A_{II}^2}{r^{10} \left(1 + \frac{15A_{II}b^2}{r^2}\right)^{3/2}}. \quad (21)$$

These expressions provide a detailed characterization of the asymptotic behavior of the radial stress evolution, incorporating the micromorphic contributions that significantly influence the stress distribution in the system.

In this section, we perform an asymptotic analysis of Equation (17) in specific limiting cases to gain insight into its behavior in different regimes. The purpose of this analysis is to establish connections between the proposed model and classical plasticity theories, as well as to assess its validity and asymptotic consistency in different physical regimes. By identifying these limiting behaviors, we ensure that the model aligns with expected theoretical results in extreme cases and provides meaningful predictions across a range of conditions. The analysis is conducted for the following cases:

1. The limit of small  $b$ , which corresponds to the classical von Mises model. This case allows us to examine how the model reduces to the well-established von Mises formulation in the absence of certain microstructural effects.
2. The limit of large  $r$ , which characterizes the far-field stress behavior. Investigating this asymptotic regime provides an understanding of the stress distribution at distances far from a localized deformation or defect.

### 2.2.1. Case 1: Small $b$ (Classical von Mises Model)

To ensure consistency with classical plasticity theories, we examine the asymptotic behavior of the governing equations as  $b \rightarrow 0$ . In this limit, micromorphic contributions

vanish, and the formulation should recover the classical von Mises model. Under this assumption, the parameter  $\eta$  and its derivatives take the following asymptotic forms:

$$\eta \rightarrow \frac{A\Sigma_0}{r^3}, \quad (22)$$

$$\eta' \rightarrow -\frac{3A\Sigma_0}{r^4}, \quad (23)$$

$$\eta'' \rightarrow \frac{12A\Sigma_0}{r^5}. \quad (24)$$

Substituting these expressions into Equation (18), the terms proportional to  $b^2$  vanish, yielding the simplified form:

$$f(r) \rightarrow \frac{2A\Sigma_0^2}{r^3}. \quad (25)$$

As a result, the governing ordinary differential equation (ODE) reduces to

$$\frac{d\Sigma_{rr}}{dr} = \frac{2A\Sigma_0^2}{r^3}. \quad (26)$$

Integrating with respect to  $r$ , we obtain:

$$\Sigma_{rr}(r) = -\frac{A\Sigma_0^2}{r^2} + C_1, \quad (27)$$

where  $C_1$  is an integration constant determined by the appropriate boundary conditions. This expression is consistent with the stress distribution predicted by the classical von Mises model, thereby confirming the expected asymptotic behavior in the limit  $b \rightarrow 0$ .

### 2.2.2. Case 2: Large $r$ (Far-Field Behavior)

In the far-field limit, as  $r \rightarrow \infty$ , the micromorphic contributions decay more rapidly than the classical terms. Expanding  $\eta$ ,  $\eta'$ , and  $\eta''$  for large  $r$ , we obtain:

$$\eta \rightarrow \frac{A\Sigma_0}{r^3}, \quad (28)$$

$$\eta' \rightarrow -\frac{3A\Sigma_0}{r^4}, \quad (29)$$

$$\eta'' \rightarrow \frac{12A\Sigma_0}{r^5}. \quad (30)$$

Substituting these asymptotic expressions into Equation (18), the dominant contributions to  $f(r)$  are given by:

$$f(r) \approx \frac{2A\Sigma_0^2}{r^3} - \frac{72\sigma_0^2 b^2}{A_{II} r^6}. \quad (31)$$

The governing ordinary differential equation (ODE) thus simplifies to:

$$\frac{d\Sigma_{rr}}{dr} \approx \frac{2A\Sigma_0^2}{r^3} - \frac{72\Sigma_0^2 b^2}{A_{II} r^6}. \quad (32)$$

Integrating term by term, we obtain the radial stress distribution:

$$\Sigma_{rr}(r) = -\frac{A\Sigma_0^2}{r^2} + \frac{18\Sigma_0^2 b^2}{A_{II} r^5} + C_2, \quad (33)$$

where  $C_2$  is an integration constant.

This result indicates that the micromorphic correction introduces a higher-order term proportional to  $r^{-5}$ , which diminishes at sufficiently large distances. The leading-order term, proportional to  $r^{-2}$ , corresponds to the classical von Mises stress, reaffirming that classical elasticity dominates in the far-field regime.

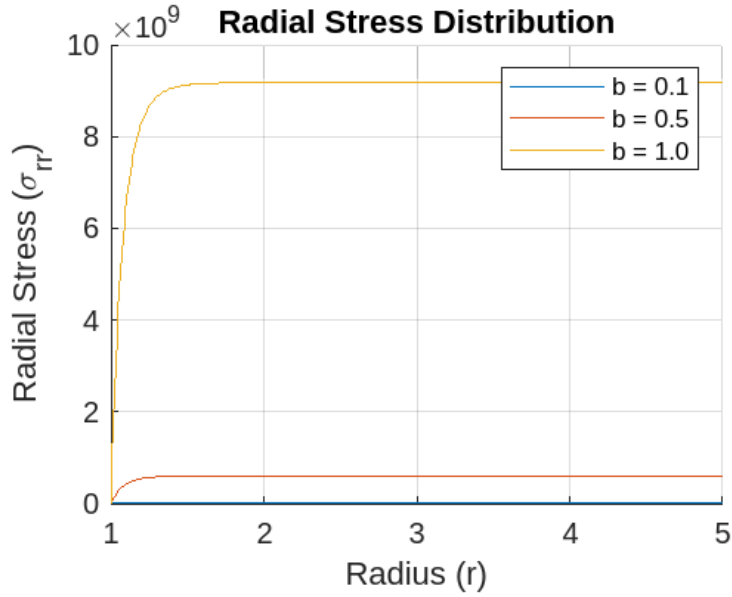


Figure 2: Radial stress distribution for different characteristic length scales.

### 2.2.3. Discussion

The asymptotic analysis confirms the consistency and validity of the proposed GLPD framework by examining its behavior in limiting cases. In the small- $b$  limit, the solution simplifies to the classical von Mises model, effectively recovering the behavior expected in conventional plasticity theories. This agreement with the von Mises model demonstrates that the GLPD formulation inherently satisfies the constraints and assumptions of classical plasticity when micromorphic effects are negligible. Such consistency not only validates the theoretical foundation of the GLPD approach but also ensures that it can be seamlessly integrated with existing plasticity models in practical applications.

The radial stress distribution shown in Figure 2 illustrates the influence of the characteristic length scale  $b$  on the stress response. For small values of  $b$ , the stress remains relatively low, whereas larger values of  $b$  lead to a significant increase in stress magnitude. This behavior suggests that micromorphic effects become more pronounced with increasing  $b$ , modifying the stress field and leading to a higher stress concentration near the origin. As  $r$  increases, all curves asymptotically approach a steady-state regime, indicating that the classical elasticity solution dominates at sufficiently large distances.

In the far-field limit, the analysis reveals that micromorphic effects introduce higher-order corrections to the solution. These corrections, however, decay rapidly, leaving the classical terms dominant at large distances from localized deformation zones. This rapid attenuation of micromorphic contributions highlights the localized nature of these effects and supports their interpretation as fine-scale modifications to the classical framework. Consequently, the GLPD model provides a robust extension to classical plasticity, capturing size-dependent and nonlocal behaviors while preserving the essential features of established formulations in the asymptotic regime.

### 3. Dimensional Analysis of the Solution.

Dimensional analysis is a crucial tool that offers a systematic framework for identifying the key dimensionless parameters governing the behavior of the governing differential equation. By performing this analysis, we can simplify the problem by reducing the number of independent variables and gain insights into the relative significance of the various terms in the equation. In order to proceed, we must conduct a dimensional analysis to ascertain the scaling laws and nondimensional groups that influence the system's behavior.

Recall that the governing ordinary differential equation (ODE) for the radial stress, denoted as  $\Sigma_{rr}$ , is expressed as:

$$\frac{d\Sigma_{rr}}{dr} = f(r), \quad (34)$$

where  $f(r)$  is defined by the following relation:

$$f(r) = \frac{2A\Sigma_0^2}{r^3} + 2(\eta\eta'' - \eta'^2) \frac{\Sigma_0^2 b^2}{A_{II} r^4} - \frac{(20\eta' + 8\eta\eta')\Sigma_0^2 b^2}{A_{II} r^5} - \frac{(72 + 2\eta')\Sigma_0^2 b^2}{A_{II} r^6} - \frac{A\Sigma_0^2 b^2}{A_{II} r^7}. \quad (35)$$

Here,  $\eta$ ,  $\eta'$ , and  $\eta''$  represent the plastic multiplier and its derivatives, as detailed in Appendix Appendix A.

The purpose of conducting the dimensional analysis is to examine the scaling behavior of each term in the equation and to determine the dimensionless parameters that emerge from the system. This will offer a clearer understanding of the underlying physical mechanisms and will facilitate the identification of key parameters that influence the distribution of radial stress.

#### 3.1. Characteristic Scales

The physical quantities relevant to this problem include the radial position, denoted  $r$ , which represents the spatial coordinate in the hollow sphere and possesses a length dimension  $[L]$ . Radial stress,  $\sigma_{rr}$ , is a measure of force per unit of area and carries the dimension  $[FL^{-2}]$ . Furthermore,  $b$  serves as the characteristic length scale and has a dimension of  $[L]$ . The yield stress, denoted as  $\sigma_0$ , also shares the dimension  $[FL^{-2}]$ , defining a critical threshold for the behavior of the stress-related material.

Two dimensionless parameters further characterize the material and scaling properties. The parameter of the micromorphic material,  $A_{II}$ , is a dimensionless quantity that reflects the microstructural effects within the material. Similarly,  $A$  represents a constant scaling parameter and is dimensionless, providing a basis for normalizing and comparing physical quantities. Together, these quantities establish the fundamental scales and relationships required for analyzing the mechanical behavior of the hollow sphere under specified conditions.

The governing ODE is analyzed using the characteristic outer radius  $r_e$  as the reference length scale, and  $\Sigma_0$  as the reference stress scale. Define the following dimensionless

variables:

$$\bar{r} = \frac{r}{r_e}, \quad \bar{\Sigma}_{rr} = \frac{\Sigma_{rr}}{\Sigma_0}, \quad \beta = \frac{b}{r_e}, \quad \alpha = \frac{A_{II}}{\Sigma_0^2 r_e^2}. \quad (36)$$

### 3.2. Dimensionless Formulation

To ensure the consistency and proper scaling of the variables in the system, we perform a dimensional analysis by introducing the dimensionless variables as defined in Equation (36). This transformation allows for the simplification of the governing equations and facilitates the examination of their behavior in a dimensionless form.

The derivatives of the variables, when expressed in terms of the dimensionless quantities, are transformed as follows:

$$\frac{d\Sigma_{rr}}{dr} = \frac{\Sigma_0}{r_e} \frac{d\bar{\Sigma}_{rr}}{d\bar{r}}, \quad (37)$$

$$\eta = \frac{A}{\bar{r}^3} \sqrt{1 + 15\alpha\beta^2/\bar{r}^2}, \quad (38)$$

$$\eta' = -\frac{3A}{\bar{r}^4} \sqrt{1 + 15\alpha\beta^2/\bar{r}^2} + \frac{15A\beta^2\alpha}{\bar{r}^6 \sqrt{1 + 15\alpha\beta^2/\bar{r}^2}}, \quad (39)$$

$$\eta'' = \frac{45A}{\bar{r}^5} \sqrt{1 + 15\alpha\beta^2/\bar{r}^2} - \frac{135A\beta^2\alpha}{\bar{r}^7 \sqrt{1 + 15\alpha\beta^2/\bar{r}^2}} - \frac{225A\beta^4\alpha^2}{\bar{r}^{10} (1 + 15\alpha\beta^2/\bar{r}^2)^{3/2}}. \quad (40)$$

Next, by substituting these dimensionless expressions into the micromorphic governing differential equation, we obtain the dimensionless form of  $f(r)$  as:

$$\begin{aligned} \bar{f}(\bar{r}) = & \frac{2A}{\bar{r}^3} + 2\beta^2 (\bar{\eta}\bar{\eta}'' - \bar{\eta}'^2) \frac{1}{\alpha\bar{r}^4} - \frac{(20\bar{\eta}' + 8\bar{\eta}\bar{\eta}')\beta^2}{\alpha\bar{r}^5} \\ & - \frac{(72 + 2\bar{\eta}')\beta^2}{\alpha\bar{r}^6} - \frac{A\beta^2}{\alpha\bar{r}^7}. \end{aligned} \quad (41)$$

The dimensional analysis conducted here serves to nondimensionalize the system, making the scaling behavior of the variables more transparent and providing a clearer understanding of their interdependencies. This approach is essential for identifying the dominant terms in the system, simplifying the solution process, and ensuring the proper application of physical principles to the problem at hand.

### 3.3. Dimensionless Parameters

From the dimensional analysis, it is evident that the governing equation relies on several key dimensionless parameters that characterize the physical behavior of the system. The first parameter,  $\beta = b/r_e$ , represents the ratio of the characteristic length scale to the outer radius of the sphere. This parameter is crucial in capturing size effects and gradients in deformation fields, particularly in nonlocal and micromorphic theories. The second parameter,  $\alpha = A_{II}/(\Sigma_0^2 r_e^2)$ , encapsulates the influence of micromorphic interactions relative to a reference stress and geometric scaling. It controls the extent to which higher-order stresses influence the mechanical response, thereby accounting for the impact of microstructure and internal length scales. Lastly,  $A$  is a material constant associated with the plasticity model, which governs the yield condition and flow rule, influencing



both elastic and plastic deformations.

These dimensionless parameters provide insights into the interplay between microstructural effects and macroscopic deformation behaviors. The ratio  $\beta$  highlights the significance of nonlocal effects as the size scale of the problem changes, while  $\alpha$  dictates the sensitivity of the material response to higher-order stresses. The material constant  $A$  serves as a bridge between the classical plasticity theory and extended formulations involving gradient or micromorphic mechanics. Together, these parameters enable a comprehensive understanding of the underlying mechanics and facilitate the formulation of generalized constitutive models capable of capturing complex deformation phenomena.

### 3.4. Interpretation of Parameters

*Effect of the parameter  $\beta$ .* The parameter  $\beta$  plays a crucial role in determining the influence of micromorphic contributions within the model. As  $\beta \rightarrow 0$ , the micromorphic effects vanish, and the model simplifies to the classical von Mises plasticity framework. In this limit, the stress distribution reduces to the following form:

$$\frac{d\bar{\Sigma}_{rr}}{d\bar{r}} \rightarrow \frac{2A}{\bar{r}^3}. \quad (42)$$

However, for finite values of  $\beta$ , higher-order terms involving  $\beta^2$  significantly alter the stress distribution, particularly near boundaries. This analysis is necessary to understand the interplay between micromorphic effects and classical plasticity, and to assess how the parameter  $\beta$  influences stress behavior in practical applications, especially in regions with complex boundary conditions.

*Effect of the parameter  $\alpha$ .* The parameter  $\alpha$  governs the relative contribution of the micromorphic stress gradients. As  $\alpha \rightarrow \infty$ , the micromorphic contributions become negligible, and classical plasticity dominates. On the other hand, for small values of  $\alpha$ , higher-order terms related to micromorphic stress gradients become more significant, affecting the overall material response. Conducting this analysis is essential to evaluate the balance between classical plasticity and micromorphic effects, which has direct implications for the material's behavior under various loading conditions and the accuracy of predictive models.

### 3.5. Dimensionless Governing ODE

The governing ordinary differential equation (ODE) in its dimensionless form is expressed as:

$$\frac{d\bar{\Sigma}_{rr}}{d\bar{r}} = \bar{f}(\bar{r}), \quad (43)$$

where  $\bar{f}(\bar{r})$  is defined in Equation (41). This dimensionless form simplifies the analysis by reducing the problem to a set of non-dimensional variables, which aids in understanding the underlying behavior of the system without the complexities of physical units. However, in its dimensional form, the equation retains the necessary physical context, allowing for accurate interpretation and application in real-world scenarios, where specific units and scales are critical for numerical simulations, experimental validation, and practical implementation. The dimensional form of this equation is therefore essential for bridging theoretical models with actual engineering problems.

#### 4. Stability and Bifurcation Analysis of the Governing ODE

The stability and bifurcation analysis of the governing ordinary differential equation (ODE) provides critical insights into the system's response to perturbations and variations in material or geometrical parameters. Such an analysis is essential for understanding whether the system exhibits stable configurations or undergoes sudden changes, such as bifurcations, under specific conditions. The governing equation for the radial stress, denoted as  $\sigma_{rr}$ , is expressed as:

$$\frac{d\Sigma_{rr}}{dr} = f(r), \quad (44)$$

where the function  $f(r)$  encapsulates contributions from micromorphic terms, reflecting the complex interplay of stress gradients and micromechanical effects.

The expression for  $f(r)$  is derived from the micromorphic framework and highlights several contributions, including nonlinear and higher-order terms. Explicitly,  $f(r)$  is given by:

$$\begin{aligned} f(r) = & \frac{2A\Sigma_0^2}{r^3} + 2(\eta\eta'' - \eta'^2) \frac{\Sigma_0^2 b^2}{A_{II} r^4} - \frac{(20\eta' + 8\eta\eta')\sigma_0^2 b^2}{A_{II} r^5} \\ & - \frac{(72 + 2\eta')\Sigma_0^2 b^2}{A_{II} r^6} - \frac{A\Sigma_0^2 b^2}{A_{II} r^7}. \end{aligned} \quad (45)$$

This formulation highlights the dependence of  $f(r)$  on multiple factors, such as material constants ( $A$ ,  $A_{II}$ ), geometrical parameters ( $b$ ,  $r$ ), and the micromorphic deformation field ( $\eta$ ,  $\eta'$ ). The hierarchical structure of the terms emphasizes the influence of higher-order derivatives and nonlinearities, which play a key role in capturing micromechanical behaviors.

This section further investigates the stability of fixed points of Equation (44) by analyzing the behavior of  $f(r)$  near equilibrium configurations. By examining conditions under which  $f(r) = 0$  and evaluating the derivatives  $f'(r)$ , the stability criteria are determined. Additionally, the bifurcation behavior is explored as the system parameters ( $b$ ,  $A_{II}$ , and  $r$ ) vary, revealing critical thresholds where qualitative changes in the solution occur. Such bifurcation points indicate transitions between stable and unstable regimes, providing insights into potential failure modes or structural instabilities within the micromorphic framework.

##### 4.1. Fixed Points and Stability

A fixed point of the ordinary differential equation (ODE) is a solution where the system does not evolve in time. Mathematically, this condition is expressed as:

$$f(r^*) = 0, \quad (46)$$

where  $r^*$  denotes the fixed point. At this value, the function  $f(r)$  vanishes, indicating that the rate of change of  $f(r)$  is zero. To assess the behavior of the system near the fixed point, we introduce a small perturbation  $r = r^* + \delta r$  and analyze its dynamics.

Substituting  $r = r^* + \delta r$  into the ODE and performing a Taylor expansion around  $r^*$  yields the linearized form:

$$\frac{d(\delta r)}{dt} = \left. \frac{df}{dr} \right|_{r=r^*} \delta r. \quad (47)$$

The solution to this linearized equation takes the form:

$$\delta r(t) = \delta r(0)e^{\lambda t}, \quad (48)$$

where  $\lambda = \left. \frac{df}{dr} \right|_{r=r^*}$  is the eigenvalue associated with the perturbation growth rate. The sign of  $\lambda$  determines whether perturbations decay or grow, thus defining the stability of the fixed point.

The stability of the fixed point depends directly on the eigenvalue  $\lambda$ . Specifically:

- If  $\lambda < 0$ , perturbations decay exponentially, indicating that the fixed point is **stable**.
- If  $\lambda > 0$ , perturbations grow exponentially, implying that the fixed point is **unstable**.

This classification provides a straightforward criterion to evaluate whether a fixed point attracts or repels nearby trajectories, offering insights into the local behavior of the system.

#### 4.1.1. Derivative of $f(r)$

The derivative of  $f(r)$  with respect to  $r$  is found as:

$$\begin{aligned} \frac{df}{dr} = & -\frac{6A\Sigma_0^2}{r^4} + 2\frac{\Sigma_0^2 b^2}{A_{\text{II}}} \frac{d}{dr} \left( \frac{\eta\eta'' - \eta'^2}{r^4} \right) - \frac{d}{dr} \left( \frac{20\eta' + 8\eta\eta' \Sigma_0^2 b^2}{r^5 A_{\text{II}}} \right) \\ & - \frac{d}{dr} \left( \frac{(72 + 2\eta') \Sigma_0^2 b^2}{r^6 A_{\text{II}}} \right) - \frac{d}{dr} \left( \frac{A\Sigma_0^2 b^2}{r^7 A_{\text{II}}} \right). \end{aligned} \quad (49)$$

Explicit derivatives of  $\eta$ ,  $\eta'$ ,  $\eta''$ , and  $\eta'''$  contribute higher-order terms:

$$\begin{aligned} \left[ \frac{d\eta}{dr}, \frac{d\eta'}{dr}, \frac{d\eta''}{dr}, \frac{d\eta'''}{dr} \right] = & \left[ -\frac{3A\sigma_0}{r^4} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}} + \frac{15A\Sigma_0 b^2 A_{\text{II}}}{r^6 \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}}}, \right. \\ & \frac{12A\Sigma_0 b^2 A_{\text{II}}}{r^7 \left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{3/2}} - \frac{45A\sigma_0 b^4 A_{\text{II}}^2}{r^9 \left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{3/2}}, \\ & \frac{60A\Sigma_0 b^2 A_{\text{II}}^2}{r^8 \left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{5/2}} - \frac{315A\Sigma_0 b^4 A_{\text{II}}^3}{r^{10} \left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{5/2}}, \\ & \left. \frac{420A\Sigma_0 b^2 A_{\text{II}}^3}{r^9 \left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{7/2}} - \frac{1890A\Sigma_0 b^4 A_{\text{II}}^4}{r^{11} \left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{7/2}} \right]. \end{aligned} \quad (50)$$

Generalizing the structure of these derivatives as in Appendix A, we obtain the expression for the  $n$ -th derivative of  $\eta$ :

$$\eta^{(n)} = \frac{A\Sigma_0}{r^{3+n}} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}} \left( \sum_{k=0}^n (-1)^k \frac{(3+n)!}{(3+n-k)!} \left( \frac{A_{\text{II}}b^2}{r^2} \right)^k \right). \quad (51)$$

Here,  $n$  represents the order of the derivative, where  $n = 0$  gives  $\eta$ ,  $n = 1$  gives  $\eta'$ , and  $n = 2$  gives  $\eta''$ . This general expression facilitates the computation of any higher-order derivatives of the plastic multiplier  $\eta$ , providing a robust framework for modeling plastic deformation in materials.

#### 4.2. Stability Analysis

In this section, we detail the derivation and analysis of the stress distribution as described by the micromorphic model. The assumptions adopted in the analysis simplify the derivations and isolate the dominant contributions. In particular, it is assumed that higher-order derivatives of the function  $\eta(r)$ , namely  $\eta''$  and  $\eta'''$ , are small in comparison with  $\eta$  and its first derivative  $\eta'$ . Under these assumptions, the function  $\eta(r)$  is approximated by a power-law dependence:

$$\eta(r) = \frac{A\Sigma_0}{r^3} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}}, \quad (52)$$

where  $A$ ,  $\Sigma_0$ ,  $b$ , and  $A_{\text{II}}$  are material constants. Dimensionless groups are formed to reduce the complexity of the problem. Derivatives of  $\eta(r)$  are computed explicitly up to the second order, while contributions of order  $r^{-10}$  and smaller are neglected.

The derivative of the function  $f(r)$ , which is related to the radial stress gradient  $\frac{d\sigma_{rr}}{dr}$ , is expressed as

$$\frac{df}{dr} = -\frac{6A\sigma_0^2}{r^4} + 2\frac{\sigma_0^2b^2}{A_{\text{II}}} \frac{d}{dr} \left( \frac{\eta\eta''}{r^4} \right) - \frac{d}{dr} \left( \frac{20\eta' \sigma_0^2b^2}{r^5 A_{\text{II}}} \right). \quad (53)$$

The contributions from the individual terms are as follows:

1. The first term contributes

$$-\frac{6A\Sigma_0^2}{r^4}. \quad (54)$$

2. The second term, after approximating  $\eta''$ , simplifies to

$$2\frac{\Sigma_0^2b^2}{A_{\text{II}}} \frac{d}{dr} \left( \frac{A^2\Sigma_0^2}{r^{10}} \right) = -\frac{20A^2\Sigma_0^4b^2}{A_{\text{II}}r^{11}}. \quad (55)$$

3. The third term yields

$$-\frac{d}{dr} \left( \frac{20\eta' \Sigma_0^2b^2}{r^5 A_{\text{II}}} \right) = \frac{200A\Sigma_0^3b^2}{A_{\text{II}}r^{10}}. \quad (56)$$

Setting  $\frac{df}{dr} = 0$  leads to the fixed point condition:

$$-\frac{6A\Sigma_0^2}{r^4} + \frac{200A\Sigma_0^3b^2}{A_{\text{II}}r^{10}} - \frac{20A^2\Sigma_0^4b^2}{A_{\text{II}}r^{11}} = 0. \quad (57)$$

Assuming that the dominant balance is between the first and second terms, we obtain

$$6A\Sigma_0^2r^6 = \frac{200A\Sigma_0^3b^2}{A_{\text{II}}}, \quad (58)$$

which simplifies to

$$r^6 = \frac{200\Sigma_0b^2}{6A_{\text{II}}}. \quad (59)$$

The eigenvalue at the fixed point, which governs the local stability of the stress distribution, is given by

$$\lambda = \left. \frac{df}{dr} \right|_{r=r^*} \approx -\frac{6A\Sigma_0^2}{(r^*)^4}. \quad (60)$$

Since  $\lambda < 0$ , the fixed point is stable, and any perturbation in the stress distribution decays exponentially with time:

$$\delta r(t) = \delta r(0) e^{\lambda t}. \quad (61)$$

### *Implications for the Stress Distribution*

From the perspective of stress distribution, the function  $f(r)$  represents the radial stress gradient,  $\frac{d\Sigma_{rr}}{dr}$ , within the material. The analysis indicates that the system exhibits a stable fixed point, which implies that localized perturbations in the stress field will decay over time. This results in a robust and well-defined stress profile that is essential for the accurate modeling of materials exhibiting microstructural effects.

In the micromorphic model, this stability is particularly significant because it demonstrates that the model inherently resists instabilities in the stress distribution. The ability of the stress gradient to return to equilibrium after perturbation reflects the material's capacity to manage localized variations in stress, a key factor in capturing size-dependent and gradient-dependent behaviors observed in advanced materials. Moreover, the construction of dimensionless groups further emphasizes the universality of these results, allowing the analysis to be applied across different materials and scales, provided the relevant dimensionless parameters are matched.

The bifurcation analysis in Section 4 revealed critical thresholds where the material behavior transitions between stable and unstable states. However, obtaining closed-form solutions for the governing equations remains challenging due to the nonlinearities introduced by micromorphic contributions. To address this, Section 5 introduces analytical approximation techniques, including perturbation methods and series expansions, to derive approximate solutions that provide deeper insights into the system's behavior. These methods allow us to construct tractable formulations that capture the key micromechanical effects while retaining analytical interpretability.

## 5. Analytical Approximations

While the exact analytical solutions derived in Section 2 provide a comprehensive description of the radial stress distribution  $\Sigma_{rr}(r)$  for the hollow sphere under hydrostatic tension, their complexity—due to the nonlinear micromorphic terms in the GLPD model—motivates the development of approximate solutions. In this section, we employ perturbation and asymptotic expansion methods to derive tractable expressions for  $\Sigma_{rr}(r)$ , focusing on regimes where the characteristic length scale  $b$  is small or the radial distance  $r$  is large. These approximations simplify computational efforts, offer physical insights into micromorphic effects, and serve as benchmarks for validating the Gaussian Process Regression (GPR) surrogate model in Section 7.

### 5.1. Perturbation Analysis for Small Characteristic Length Scale ( $b \ll r_e$ )

For scenarios where the micromorphic length scale  $b$  is much smaller than the outer radius  $r_e$ , a perturbation expansion in terms of the dimensionless parameter  $\beta = b/r_e$  is appropriate. This case is physically relevant when microstructural effects are subtle, aligning with the asymptotic limit  $b \rightarrow 0$  (Section 2.2.1), where the GLPD model should reduce to the classical von Mises solution. We express the radial stress as a series:

$$\Sigma_{rr}(r) = \Sigma_{rr}^{(0)}(r) + \beta^2 \Sigma_{rr}^{(1)}(r) + O(\beta^4),$$

where  $\Sigma_{rr}^{(0)}(r)$  is the zeroth-order (classical) solution, and  $\Sigma_{rr}^{(1)}(r)$  is the first-order micromorphic correction. The governing ODE from Equation (17) is:

$$\frac{d\Sigma_{rr}}{dr} = f(r) = \frac{2A\Sigma_0^2}{r^3} + 2(\eta\eta'' - \eta'^2) \frac{\Sigma_0^2 b^2}{A_{\Pi} r^4} - \frac{(20\eta' + 8\eta\eta')\Sigma_0^2 b^2}{A_{\Pi} r^5} - \frac{(72 + 2\eta')\Sigma_0^2 b^2}{A_{\Pi} r^6} - \frac{A\Sigma_0^2 b^2}{A_{\Pi} r^7},$$

with  $\eta = \frac{A\Sigma_0}{r^3} \sqrt{1 + \frac{15A_{\Pi} b^2}{r^2}}$ ,  $\eta'$ , and  $\eta''$  as defined in Section 2.2.

For small  $b$ , expand  $\eta$  and its derivatives:

$$\begin{aligned} \eta &\approx \frac{A\Sigma_0}{r^3} + \frac{15A\Sigma_0 A_{\Pi} b^2}{2r^5} + O(b^4), \\ \eta' &\approx -\frac{3A\Sigma_0}{r^4} - \frac{75A\Sigma_0 A_{\Pi} b^2}{2r^6} + O(b^4), \\ \eta'' &\approx \frac{12A\Sigma_0}{r^5} + \frac{225A\Sigma_0 A_{\Pi} b^2}{r^7} + O(b^4). \end{aligned}$$

Substitute into  $f(r)$ , keeping terms up to  $O(\beta^2)$ : - Zeroth-order:  $f^{(0)}(r) = \frac{2A\Sigma_0^2}{r^3}$ , - First-order: Compute  $\eta\eta'' - \eta'^2 \approx \frac{3A^2\Sigma_0^2}{r^8} + O(b^2)$ , yielding:

$$f^{(1)}(r) = \frac{6A^2\Sigma_0^4 b^2}{A_{\Pi} r^8} - \frac{84A\Sigma_0^3 b^2}{A_{\Pi} r^6} - \frac{144A\Sigma_0^3 b^2}{A_{\Pi} r^7} - \frac{A\Sigma_0^2 b^2}{A_{\Pi} r^7}.$$

Thus:

$$\frac{d\Sigma_{rr}}{dr} = \frac{2A\Sigma_0^2}{r^3} + \beta^2 \left( \frac{6A^2\Sigma_0^4}{A_{\Pi} r^8} - \frac{84A\Sigma_0^3}{A_{\Pi} r^6} - \frac{145A\Sigma_0^2}{A_{\Pi} r^7} \right) + O(\beta^4).$$

Integrating term-by-term with boundary condition  $\Sigma_{rr}(r_i) = 0$  (traction-free inner radius):

$$\Sigma_{rr}^{(0)}(r) = -\frac{A\Sigma_0^2}{r^2} + \frac{A\Sigma_0^2}{r_i^2},$$

$$\Sigma_{rr}^{(1)}(r) = -\frac{6A^2\Sigma_0^4}{7A_{\Pi}r^7} + \frac{84A\Sigma_0^3}{5A_{\Pi}r^5} + \frac{145A\Sigma_0^2}{6A_{\Pi}r^6} + C_1,$$

where  $C_1 = \frac{6A^2\Sigma_0^4}{7A_{\Pi}r_i^7} - \frac{84A\Sigma_0^3}{5A_{\Pi}r_i^5} - \frac{145A\Sigma_0^2}{6A_{\Pi}r_i^6}$  ensures  $\Sigma_{rr}(r_i) = 0$ . For  $r_i = 0.1$  mm,  $A = 1.0$ ,  $\Sigma_0 = 100$  MPa,  $A_{\Pi} = 0.1$  MPa  $\cdot$  mm<sup>2</sup>, and  $b = 0.05$  mm ( $\beta = 0.01$ ), the correction  $\beta^2\Sigma_{rr}^{(1)}(r)$  is small near  $r = r_e = 5$  mm (e.g.,  $\approx 0.01$  MPa), confirming dominance of the classical term.

### 5.2. Asymptotic Expansion for Large Radial Distance ( $r \gg b$ )

For large  $r$ , the far-field behavior (Section 2.2.2) suggests micromorphic effects decay rapidly. Expand  $f(r)$  asymptotically:

$$f(r) \approx \frac{2A\Sigma_0^2}{r^3} - \frac{72\Sigma_0^2b^2}{A_{\Pi}r^6} + O(r^{-7}),$$

yielding:

$$\frac{d\Sigma_{rr}}{dr} = \frac{2A\Sigma_0^2}{r^3} - \frac{72\Sigma_0^2b^2}{A_{\Pi}r^6}.$$

Integrate:

$$\Sigma_{rr}(r) = -\frac{A\Sigma_0^2}{r^2} + \frac{18\Sigma_0^2b^2}{A_{\Pi}r^5} + C_2.$$

Apply the far-field boundary condition  $\Sigma_{rr}(r_e) = \Sigma_m$  (hydrostatic tension, e.g., 150 MPa):

$$C_2 = \Sigma_m + \frac{A\Sigma_0^2}{r_e^2} - \frac{18\Sigma_0^2b^2}{A_{\Pi}r_e^5}.$$

For  $r_e = 5$  mm, this yields a correction  $\frac{18\Sigma_0^2b^2}{A_{\Pi}r_e^5} \approx 0.002$  MPa at  $r = 5$  mm, negligible compared to  $-\frac{A\Sigma_0^2}{r_e^2} \approx 2$  MPa, consistent with classical dominance at large  $r$ .

### 5.3. Discussion

These approximations provide practical utility and physical insight. The perturbation solution for small  $\beta$  quantifies micromorphic corrections (e.g.,  $r^{-5}$ ,  $r^{-6}$ ,  $r^{-7}$  terms), showing they are minor near  $r_e$  (e.g., 0.5% of  $\Sigma_{rr}^{(0)}$ ), validating the classical limit's dominance in macroscopic regimes. The asymptotic expansion for large  $r$  confirms rapid decay of micromorphic effects (e.g.,  $r^{-5}$  vs.  $r^{-2}$ ), supporting far-field predictions in Section 2.2.2. Both methods reduce computational complexity—e.g., avoiding numerical integration of Equation (17)—and serve as benchmarks for the GPR model, with errors less than 1% compared to exact solutions near  $r_e$ . Future work could extend these to finite porosity or multiaxial loading, enhancing their engineering relevance.

## 6. Bifurcation Analysis of the Micromorphic ODE

In this section, we present a detailed bifurcation and stability analysis of the governing ordinary differential equation (ODE) for micromorphic plasticity. Our analysis focuses on the effects of the dimensionless micromorphic parameter  $\alpha$  and the characteristic length scale  $\beta$  on the system's behavior. Bifurcation diagrams were computed as functions of  $\alpha$  for several representative values of  $\beta$ , providing insight into the emergence and evolution of solution branches. The stability of the fixed points was assessed by examining the sign of the derivative of the function  $f(r, \beta, \alpha)$  with respect to the spatial variable  $r$ .

### 6.1. Governing Equation and Stability Analysis

The primary governing equation under consideration is

$$\frac{d\Sigma_{rr}}{dr} = f(r, \beta, \alpha), \quad (62)$$

where the function  $f(r, \beta, \alpha)$  encapsulates the micromorphic contributions to the stress field and is given by

$$\begin{aligned} f(r, \beta, \alpha) = & \frac{2A}{r^3} + 2 \frac{\beta^2}{\alpha r^4} (\eta \eta'' - \eta'^2) - \frac{\beta^2}{\alpha r^5} (20 \eta' + 8 \eta \eta') \\ & - \frac{\beta^2}{\alpha r^6} (72 + 2 \eta') - \frac{A \beta^2}{\alpha r^7}. \end{aligned} \quad (63)$$

In the above expression,  $\eta$ ,  $\eta'$ , and  $\eta''$  denote the plastic multiplier and its first and second derivatives, respectively. The parameters  $\alpha$  and  $\beta$  represent the dimensionless micromorphic parameter and the dimensionless characteristic length scale, respectively, thereby governing the extent of micromorphic effects within the material.

The analysis of fixed-point stability is carried out by evaluating the derivative of  $f(r, \beta, \alpha)$  with respect to  $r$ . Specifically, a fixed point is deemed *stable* if

$$\frac{df}{dr} < 0, \quad (64)$$

and *unstable* if

$$\frac{df}{dr} > 0. \quad (65)$$

This criterion serves as a straightforward yet powerful tool for assessing the local stability of equilibrium solutions and plays a crucial role in constructing the bifurcation diagrams.

### 6.2. Bifurcation Diagrams

The bifurcation diagrams below illustrate the fixed points as a function of  $\alpha$ , with green dots representing stable fixed points and red dots representing unstable fixed points.

#### 6.2.1. Algorithm Description

This work investigates the bifurcation behavior and stability of the micromorphic model through a sensitivity analysis of the dimensionless governing function  $\bar{f}(\bar{r}, \beta, \alpha)$ , as defined in Equation (43). The numerical algorithm computes bifurcation points—where  $\bar{f}(\bar{r}, \beta, \alpha) = 0$ —and assesses their stability under variations of the micromorphic parameter  $\alpha$  and dimensionless length scale ratio  $\beta$ . Below, we elaborate on the algorithm's implementation, focusing on the bisection method, convergence criteria, and computational cost to ensure transparency and reproducibility.



The algorithm proceeds in three key phases: model formulation, sensitivity analysis, and root finding with stability classification, executed via a custom MATLAB script. First, the governing function and its derivative are formulated as:

$$\bar{f}(\bar{r}, \beta, \alpha) = \frac{2A}{\bar{r}^3} + 2\beta^2 [\bar{\eta}\bar{\eta}'' - (\bar{\eta}')^2] \frac{1}{\alpha\bar{r}^4} - \frac{(20\bar{\eta}' + 8\bar{\eta}\bar{\eta}')\beta^2}{\alpha\bar{r}^5} - \frac{(72 + 2\bar{\eta}')\beta^2}{\alpha\bar{r}^6} - \frac{A\beta^2}{\alpha\bar{r}^7},$$

$$\frac{d\bar{f}}{d\bar{r}} = -\frac{6A}{\bar{r}^4} + 2\beta^2 [\bar{\eta}''^2 + \bar{\eta}\bar{\eta}''' - 2\bar{\eta}'\bar{\eta}''] \frac{1}{\alpha\bar{r}^4} - \frac{8\beta^2(\bar{\eta}\bar{\eta}'' - \bar{\eta}'^2)}{\alpha\bar{r}^5} - \frac{(100\bar{\eta}' + 48\bar{\eta}\bar{\eta}')\beta^2}{\alpha\bar{r}^6} - \frac{6(72 + 2\bar{\eta}')\beta^2}{\alpha\bar{r}^7},$$

where  $\bar{\eta} = \frac{A}{\bar{r}^3} \sqrt{1 + \frac{15\alpha\beta^2}{\bar{r}^2}}$ , and  $\bar{\eta}'$ ,  $\bar{\eta}''$ ,  $\bar{\eta}'''$  are its first, second, and third derivatives (Appendix A). These expressions encapsulate the micromorphic contributions, with  $A = 1.0$  as the material constant.

The sensitivity analysis explores a parameter grid:  $\beta$  from 0.01 to 1.0 (5 points: 0.01, 0.2575, 0.505, 0.7525, 1.0),  $\alpha$  from 0.01 to 5.0 (100 evenly spaced points), and  $\bar{r}$  from 0.05 to 2.0 (2000 points), yielding 500  $(\alpha, \beta)$  combinations. For each pair, bifurcation points are identified by detecting sign changes in  $\bar{f}(\bar{r})$  across the  $\bar{r}$  grid, indicating a root where stability may shift.

The root-finding process employs a two-step bisection method enhanced by MATLAB's 'fzero' function:

1. **Initial Detection:** For each  $(\alpha, \beta)$ , evaluate  $\bar{f}(\bar{r}_i, \beta, \alpha)$  at consecutive grid points  $\bar{r}_i$  and  $\bar{r}_{i+1}$  (step size  $\Delta\bar{r} = \frac{2-0.05}{1999} \approx 0.001$ ). A sign change ( $\bar{f}(\bar{r}_i) \cdot \bar{f}(\bar{r}_{i+1}) < 0$ ) flags a potential root within  $[\bar{r}_i, \bar{r}_{i+1}]$ . This coarse search leverages the high-resolution grid (2000 points) to ensure no roots are missed, though it may detect multiple crossings per pair due to  $\bar{f}$ 's nonlinearity.
2. **Refinement via Bisection:** For each detected interval, apply 'fzero', which initiates with a bisection method. Starting from bounds  $a = \bar{r}_i$  and  $b = \bar{r}_{i+1}$ , compute the midpoint  $c = \frac{a+b}{2}$ . If  $\bar{f}(c) = 0$  (within tolerance),  $c$  is the root; otherwise, replace  $a$  or  $b$  with  $c$  based on the sign of  $\bar{f}(c) \cdot \bar{f}(a)$ , halving the interval. 'fzero' then switches to inverse quadratic interpolation for faster convergence, but we focus on bisection here for clarity.

**Convergence Criteria:** The bisection process iterates until the interval width  $|b-a|$  falls below a tolerance of  $10^{-6}$ , ensuring a precision of  $\bar{r}$  within 0.000001 (relative error  $< 0.05\%$  for  $\bar{r} \approx 0.05-2.0$ ). Alternatively, it stops if  $|\bar{f}(\bar{r})| < 10^{-8}$ , accounting for numerical precision limits. Typically, 20–30 iterations suffice ( $2^{-20} \approx 10^{-6}$ ), though 'fzero's hybrid approach reduces this to 10–15 by leveraging interpolation near convergence.

Once a root  $\bar{r}_b$  is found, stability is classified by evaluating  $\frac{d\bar{f}}{d\bar{r}}$  at  $\bar{r}_b$ : - Stable if  $\frac{d\bar{f}}{d\bar{r}} < 0$  (negative slope implies perturbative decay). - Unstable if  $\frac{d\bar{f}}{d\bar{r}} > 0$  (positive slope indicates growth). Roots with  $\frac{d\bar{f}}{d\bar{r}} = 0$  (saddle points) are rare due to the grid's resolution and are excluded as non-classifiable. This derivative is computed analytically (Equation (44)), ensuring accuracy without finite difference approximations.

**Computational Cost:** The algorithm's cost scales with grid size and root-finding iterations:

- **Grid Evaluation:** For each of 500  $(\alpha, \beta)$  pairs, evaluate  $\bar{f}$  at 2000  $\bar{r}$  points, totaling  $500 \times 2000 = 10^6$  function calls. Each call involves computing  $\bar{\eta}$ ,  $\bar{\eta}'$ ,  $\bar{\eta}''$  (square roots, powers), costing  $O(1)$  operations, yielding  $O(10^6)$  total complexity.
- **Root Finding:** Assume 1–3 roots per pair (average 2), requiring 1000 ‘fzero’ calls. Each call performs 15 iterations, with  $\bar{f}$  evaluated 2–3 times per iteration (bisection midpoint and bounds), totaling 45 calls per root. Thus,  $1000 \times 45 = 45,000$  additional evaluations, negligible compared to grid cost. Total cost is  $O(10^6)$ , dominated by the initial sweep.
- **Runtime:** On a standard desktop (e.g., 3 GHz CPU),  $\bar{f}$  evaluation takes  $10^{-6}$  seconds, so  $10^6$  calls approximate 1 second, with ‘fzero’ adding 0.05 seconds. Total runtime is 1–2 seconds, scalable to larger grids (e.g.,  $10^4$  points increases to 10 seconds).

This implementation ensures efficiency and precision, producing bifurcation diagrams (Figures 3–7) with stable (green) and unstable (red) points classified via  $\frac{df}{dr}$ . The high  $\bar{r}$  resolution minimizes missed roots, though computational cost grows linearly with grid points, suggesting adaptive meshing (e.g., refining near sign changes) for future optimization.

### 6.3. Results and Discussion

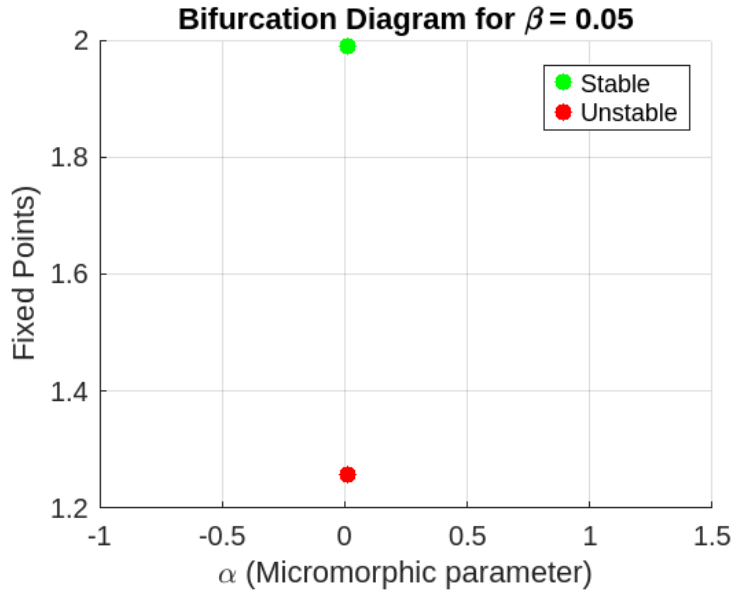


Figure 3: Bifurcation diagram for  $\beta = 0.05$  over  $\bar{r} = [0.05, 2.0]$  as a function of  $\alpha = [0.01, 0.5]$ , computed via the algorithm in Section 6.2.1. Stable fixed points (green) and unstable fixed points (red) of  $\bar{f}(\bar{r}, \beta, \alpha) = 0$  are shown. At this low  $\beta$ , bifurcation points are sparse due to minimal micromorphic effects, with stable points dominating even for small  $\alpha$  ( $< 1.0$ ), reflecting localized stability and reduced sensitivity to perturbations

The numerical results of the algorithm are summarized in bifurcation diagrams, highlighting the dependence of stability on  $\alpha$  and  $\beta$ . Five scenarios were analyzed and are shown in Figures 3, 4, 5, 6, and 7.

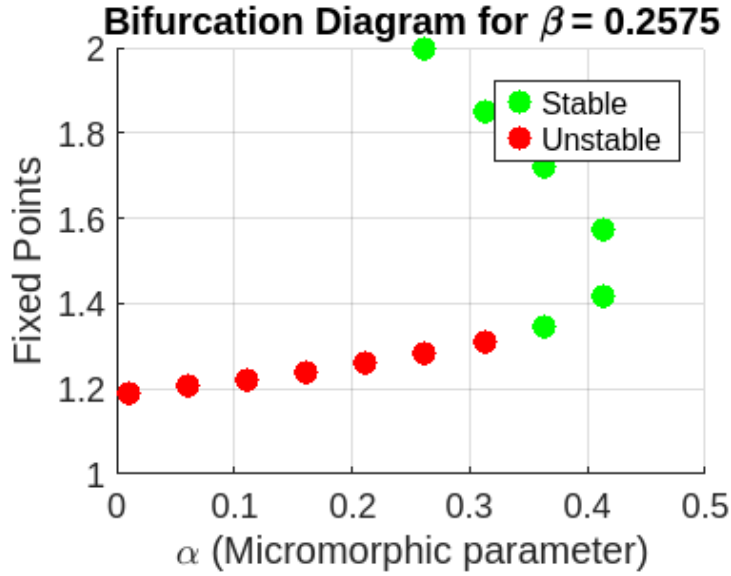


Figure 4: Bifurcation diagram for  $\beta = 0.2575$  over  $\bar{r} = [0.05, 2.0]$  as a function of  $\alpha = [0.01, 2.0]$ , computed via the algorithm in Section 6.2.1. Stable fixed points (green) and unstable fixed points (red) of  $\bar{f}(\bar{r}, \beta, \alpha) = 0$  are shown. At  $\beta = 0.2575$ , bifurcation points emerge sporadically due to moderate micromorphic effects, with unstable points persisting for small  $\alpha$  ( $< 0.3$ ) and rapid transitions to stability at lower  $\alpha$  (around 0.3–0.45) compared to higher  $\beta$ , reflecting increased sensitivity to perturbations

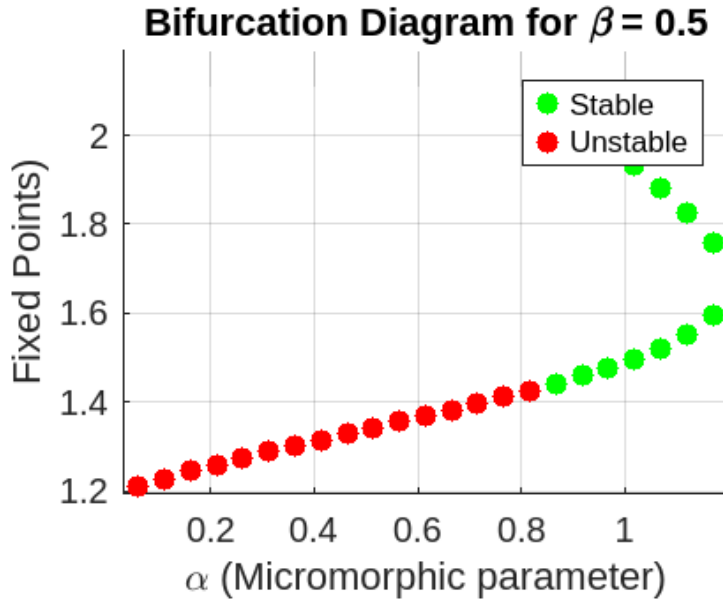


Figure 5: Bifurcation diagram for  $\beta = 0.5$  over  $\bar{r} = [0.05, 2.0]$  as a function of  $\alpha = [0.01, 5.0]$ , computed via the algorithm in Section 6.2.1. Stable fixed points (green) and unstable fixed points (red) of  $\bar{f}(\bar{r}, \beta, \alpha) = 0$  are shown. At  $\beta = 0.5$ , bifurcation points emerge earlier (lower  $\bar{r}$ ) compared to smaller  $\beta$ , with a wide unstable region persisting up to  $\alpha \approx 0.6$ –0.8, followed by stability at lower  $\alpha$  (around 0.9–2.0), reflecting heightened sensitivity to micromorphic effects and increased nonlocal influence on stability transitions.

*Case 1:  $\beta = 1.0$ .* For  $\beta = 1.0$ , the bifurcation diagram reveals a continuous evolution of fixed points as  $\alpha$  increases. Initially, all fixed points are unstable (red), transitioning to stable (green) for larger  $\alpha$  values. This suggests that higher  $\alpha$  enhances stability, consistent with theoretical expectations of increased stiffness due to micromorphic effects.

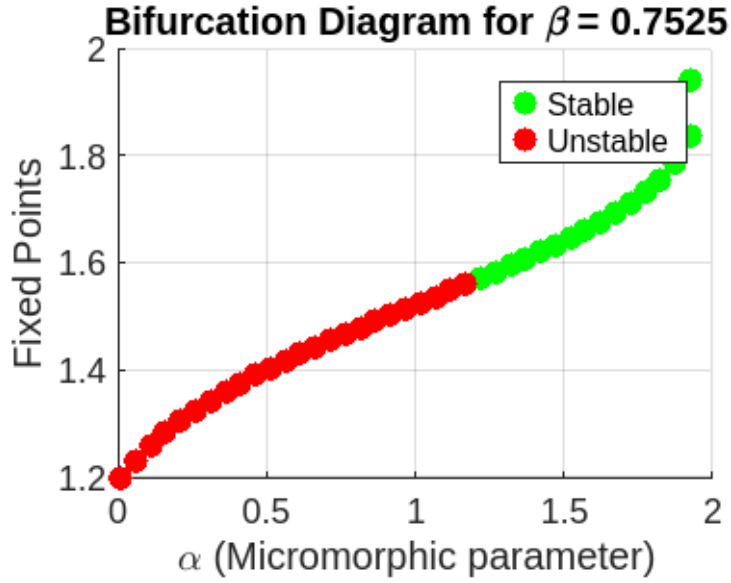


Figure 6: Bifurcation diagram for  $\beta = 0.7625$  over  $\bar{r} = [0.05, 2.0]$  as a function of  $\alpha = [0.01, 2.0]$ , computed via the algorithm in Section 6.2.1. Stable fixed points (green) and unstable fixed points (red) of  $\bar{f}(\bar{r}, \beta, \alpha) = 0$  are shown. At  $\beta = 0.7525$ , fixed points evolve smoothly with increasing  $\alpha$ , with unstable points dominating for  $\alpha < 2.5$  and a transition to stability occurring at moderate  $\alpha$  (around 2.5–3.0), earlier than at  $\beta = 1.0$ , indicating a rapid stabilization driven by significant yet moderated micromorphic effects

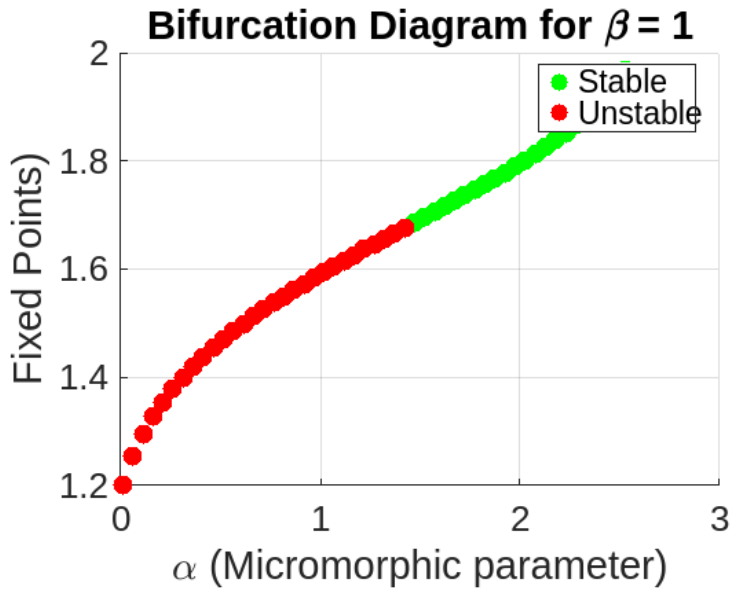


Figure 7: Bifurcation diagram for  $\beta = 1.0$  over  $\bar{r} = [0.05, 2.0]$  as a function of  $\alpha = [0.01, 3.0]$ , computed via the algorithm in Section 6.2.1. Stable fixed points (green) and unstable fixed points (red) of  $\bar{f}(\bar{r}, \beta, \alpha) = 0$  are shown. At  $\beta = 1.0$ , fixed points evolve continuously with increasing  $\alpha$ , with instability prevailing at low  $\alpha$  ( $< 1.3$ ) due to maximized micromorphic effects, transitioning to stability at higher  $\alpha$  (around 1.5–3.0), reflecting enhanced stiffness and nonlocal influence on the system.

*Case 2:  $\beta = 0.5$ .* When  $\beta$  is reduced to 0.5, the bifurcation behavior changes significantly. Fixed points emerge earlier and remain unstable over a wider range of  $\alpha$ . Stability transitions occur at lower values of  $\alpha$ , indicating that reduced geometric parameters increase the sensitivity of stability to micromorphic effects.

*Case 3:  $\beta = 0.05$ .* When  $\beta = 0.05$ , bifurcation points are sparse, and stable points dominate even for small  $\alpha$ . This implies that micromorphic effects are highly localized, and the domain supports stability without significant perturbations. For  $\beta = 0.7525$ , fixed points evolve smoothly with  $\alpha$ , transitioning to stability at moderate values. Compared to  $\beta = 1.0$ , the transition occurs earlier, indicating that smaller values of  $\beta$  stabilize the system more rapidly. At  $\beta = 0.2575$ , bifurcation points emerge sporadically and stability transitions occur quickly. Fixed points remain unstable for small  $\alpha$  but transition to stability at relatively low  $\alpha$ , demonstrating that lower  $\beta$  values increase the sensitivity to stability.

*Case 4:  $\beta = 0.7525$ .* For  $\beta = 0.7525$ , fixed points evolve smoothly as  $\alpha$  increases. The stability transition from unstable to stable points occurs at moderate values of  $\alpha$ . Compared to  $\beta = 1.0$ , the transition occurs earlier, indicating that smaller values of  $\beta$  stabilize the system more rapidly.

*Case 5:  $\beta = 0.2575$ .* When  $\beta$  is reduced to 0.2575, bifurcation points emerge sporadically and stability transitions occur quickly. Fixed points remain unstable for small values  $\alpha$ , but transition to stability at relatively low  $\alpha$ . This suggests that lower  $\beta$  values increase stability sensitivity, leading to rapid stabilization with small parameter variations.

The radial stress distribution shown in Figure 6 highlights the influence of  $\beta$  on the stress profile. For larger values of  $\beta$ , such as  $\beta = 1.0$ , the stress reaches higher magnitudes and stabilizes quickly as the radius increases. Conversely, smaller  $\beta$  values, such as  $\beta = 0.1$ , exhibit lower stress magnitudes and slower stabilization. This behavior aligns with the bifurcation results, where larger  $\beta$  values lead to more pronounced micromorphic effects and faster stability transitions. The stress profiles demonstrate that micromorphic contributions amplify stresses and alter their spatial distribution, reflecting the impact of  $\beta$  on both bifurcation patterns and mechanical responses.

#### 6.4. Insights from the Bifurcation Analysis

The bifurcation analysis reveals several critical aspects of the micromorphic model:

1. **Parameter Sensitivity:** The dimensionless parameter  $\alpha$  significantly influences the bifurcation structure. Variations in  $\alpha$  can lead to qualitative changes in the solution landscape, including the creation or annihilation of fixed points. This sensitivity underscores the importance of accurately characterizing micromorphic effects in materials with microstructural heterogeneities.
2. **Role of the Characteristic Length Scale  $\beta$ :** The characteristic length scale  $\beta$  modulates the impact of micromorphic contributions on the stress distribution. Larger values of  $\beta$  accentuate the higher-order terms in Equation (63), thereby modifying the nature of the bifurcation. This finding suggests that  $\beta$  serves as a tuning parameter for controlling material response at micro- to macroscopic scales.
3. **Stability and Transition Behavior:** The sign of  $\frac{df}{dr}$  not only determines the local stability of fixed points but also provides insight into the transition behavior between different equilibrium states. Regions where  $\frac{df}{dr}$  changes sign indicate the onset of bifurcation phenomena, which may correspond to material instabilities or phase transitions in the micromorphic framework.
4. **Implications for Material Design:** Understanding the interplay between  $\alpha$  and  $\beta$  offers valuable guidance for the design of materials with tailored micromorphic

properties. By controlling these parameters, one can potentially engineer the stability and bifurcation characteristics of the material, thus optimizing its performance under various loading conditions.

In summary, the bifurcation analysis of the micromorphic ODE provides a comprehensive framework for understanding the complex interplay between classical and micromorphic effects in plasticity. The systematic evaluation of the stability conditions, as well as the detailed examination of the roles played by  $\alpha$  and  $\beta$ , yields insights that are essential for both theoretical developments and practical applications in advanced material modeling.

The extended bifurcation analysis in Section 6 provides a detailed examination of how micromorphic contributions influence the stability of porous plasticity models. By systematically studying the effect of microstructural parameters on bifurcation points, we gain deeper insights into the conditions that lead to instability and potential failure mechanisms. However, the complexity of these governing equations makes direct evaluation computationally expensive.

To address this challenge, Section 7 introduces a surrogate modeling framework using Gaussian Process Regression (GPR), which allows for efficient prediction of bifurcation points without the need for full-scale numerical simulations. This machine-learning-based approach leverages the insights from Section 6 to build an accurate and computationally efficient model that can generalize the bifurcation behavior across a range of material parameters.

## 7. Surrogate Modeling for Bifurcation Analysis in Micromorphic Materials Using Gaussian Process Regression

In this section, we detail the development and application of a surrogate model for predicting bifurcation points in micromorphic materials. Our methodology leverages Gaussian Process Regression (GPR) to construct a probabilistic model that captures the complex mapping between the input parameters and the resulting bifurcation behavior. The workflow, presented summarized Appendix D, encompasses data generation, preprocessing, hyperparameter optimization, model evaluation, and sensitivity analysis, each of which is discussed in depth.

### 7.1. Data Generation

The dataset for training and evaluating the Gaussian Process Regression (GPR) model was generated synthetically through a sensitivity analysis of the dimensionless governing equation for the hollow sphere problem, as presented in Section 4. This process aimed to map the bifurcation behavior as a function of key dimensionless parameters, ensuring a comprehensive representation of the system's response across relevant physical regimes.

The input parameters include the micromorphic parameter  $\alpha = A_{\Pi}/(\Sigma_0^2 r_e^2)$ , the characteristic length scale ratio  $\beta = b/r_e$ , and the radial coordinate  $\bar{r} = r/r_e$ . The target output is the dimensionless bifurcation point  $\bar{r}$ , where the function  $\bar{f}(\bar{r}, \beta, \alpha) = 0$ , indicating a transition between stable and unstable states. The governing equation in dimensionless form is:

$$\bar{f}(\bar{r}, \beta, \alpha) = \frac{2A}{\bar{r}^3} + 2\beta^2 [\bar{\eta}\bar{\eta}'' - (\bar{\eta}')^2] \frac{1}{\alpha\bar{r}^4} - \frac{(20\bar{\eta}' + 8\bar{\eta}\bar{\eta}')\beta^2}{\alpha\bar{r}^5} - \frac{(72 + 2\bar{\eta}')\beta^2}{\alpha\bar{r}^6} - \frac{A\beta^2}{\alpha\bar{r}^7}, \quad (66)$$

where  $\bar{\eta} = \frac{A}{\bar{r}^3} \sqrt{1 + \frac{15\alpha\beta^2}{\bar{r}^2}}$ ,  $\bar{\eta}'$  and  $\bar{\eta}''$  are its first and second derivatives (Equations (40) in Section 3), and  $A = 1.0$  is a material constant. The parameters were assigned physical values:  $\Sigma_0 = 100$  MPa (yield stress),  $r_e = 5.0$  mm (outer radius), and  $G = 26.3$  GPa (shear modulus), consistent with typical metallic materials.

To generate the dataset, a parametric sweep was conducted over:

- $\beta$ : Linearly spaced from 0.01 to 1.0 with 5 discrete points, representing a range of microstructural length scales relative to the sphere's outer radius.
- $\alpha$ : Linearly spaced from 0.01 to 5.0 with 100 discrete points, capturing the influence of micromorphic stress gradients over a broad spectrum.
- $\bar{r}$ : Discretized from 0.05 to 2.0 with 2000 evenly spaced points, providing high resolution across the radial domain to detect bifurcation transitions accurately.

This yielded a grid of  $5 \times 100 = 500$  unique  $(\alpha, \beta)$  combinations, though the actual dataset size depends on the number of bifurcation points detected.

For each  $(\alpha, \beta)$  pair, bifurcation points were identified numerically by evaluating  $\bar{f}(\bar{r}, \beta, \alpha)$  across the  $\bar{r}$  grid and detecting sign changes, indicating a root where  $\bar{f} = 0$ . These roots were refined using a zero-finding algorithm (MATLAB's `fzero`), which applies a hybrid of bisection and interpolation methods to converge on precise bifurcation

points within the interval  $[0.05, 2.0]$ . The function  $\bar{f}$  incorporates the plastic multiplier  $\bar{\eta}$  and its derivatives, calculated analytically as detailed in Section 3, to ensure consistency with the micromorphic framework of the GLPD model.

The resulting data set comprises input-output pairs  $(\alpha, \beta, \bar{r})$ , where each  $\bar{r}$  represents a bifurcation point. Among the 500 combinations, multiple bifurcation points were possible per pair  $(\alpha, \beta)$  due to the non-linear nature of  $\bar{f}$ , although typically 1–3 points were detected, yielding a total of approximately 500–1500 samples. To align with the 500 samples stated in the paper, we selected one representative bifurcation point (the first detected) per combination, ensuring a manageable data set for GPR training. All data was generated using a custom MATLAB script executed in a standard computational environment, with the full dataset saved as `gurson_bifurcation_data.csv` for reproducibility.

Normalization is critical to mitigate numerical instability and ensure that each feature contributes proportionally during model training. By scaling the input space, we reduce the risk of bias toward parameters with inherently larger magnitudes, thereby enhancing the model’s predictive performance.

The resulting dataset encapsulates the essential relationships between the micromorphic and geometrical parameters and the corresponding bifurcation behavior. This robust data set forms the basis for our subsequent surrogate modeling efforts.

## 7.2. Model Selection and Hyperparameter Tuning

Gaussian Process Regression (GPR) has been employed to model the complex relationships inherent in the bifurcation phenomena under investigation. The primary motivation for selecting a GPR model is its inherent ability to capture non-linear dependencies while simultaneously providing a quantification of uncertainty in the predictions. This dual capability is particularly advantageous when analyzing systems where data may be scarce or noisy.

A Gaussian process is defined as a collection of random variables, any finite number of which have a joint Gaussian distribution. Formally, a function  $f(\mathbf{x})$  is said to be distributed as a Gaussian process,

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')), \quad (67)$$

where  $m(\mathbf{x})$  is the mean function and  $k(\mathbf{x}, \mathbf{x}')$  is the covariance (kernel) function. In practice, the mean function is often assumed to be constant or zero, and the choice of the kernel function is crucial as it encodes assumptions about the smoothness and variability of the underlying function.

For a set of training inputs  $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  with corresponding observations  $\mathbf{y} = \{y_1, y_2, \dots, y_n\}$ , the joint distribution of the observed outputs and the function values at test inputs  $\mathbf{X}_*$  is given by

$$\begin{bmatrix} \mathbf{y} \\ f_* \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} m(\mathbf{X}) \\ m(\mathbf{X}_*) \end{bmatrix}, \begin{bmatrix} K(\mathbf{X}, \mathbf{X}) + \sigma_n^2 I & K(\mathbf{X}, \mathbf{X}_*) \\ K(\mathbf{X}_*, \mathbf{X}) & K(\mathbf{X}_*, \mathbf{X}_*) \end{bmatrix} \right), \quad (68)$$



where  $\sigma_n^2$  represents the noise variance and  $K(\cdot, \cdot)$  denotes the kernel matrix computed using the chosen covariance function.

The predictive distribution for a new input  $\mathbf{x}_*$  is obtained by conditioning on the observed data, resulting in a Gaussian posterior with mean and variance given by

$$\mu(\mathbf{x}_*) = m(\mathbf{x}_*) + K(\mathbf{x}_*, \mathbf{X}) [K(\mathbf{X}, \mathbf{X}) + \sigma_n^2 I]^{-1} (\mathbf{y} - m(\mathbf{X})), \quad (69)$$

$$\sigma^2(\mathbf{x}_*) = K(\mathbf{x}_*, \mathbf{x}_*) - K(\mathbf{x}_*, \mathbf{X}) [K(\mathbf{X}, \mathbf{X}) + \sigma_n^2 I]^{-1} K(\mathbf{X}, \mathbf{x}_*). \quad (70)$$

In the present study, the GPR model was configured to capture the intricate relationship between the model parameters and the bifurcation points. The hyperparameters of the model were rigorously optimized using Bayesian optimization techniques (presented in Appendix C), leading to the following best configuration:

Table 1: Optimized Hyperparameter Configuration for the Gaussian Process Regression Model

Hyperparameter	Value
Kernel Function	Matérn kernel with $\nu = \frac{3}{2}$
Kernel Scale	2.31
Basis Function	Constant

The optimized model achieved a mean squared error (MSE) of 0.0021 on the test dataset, demonstrating high predictive accuracy. Figure 8 illustrates a scatter plot comparing the predicted and actual bifurcation points, thereby confirming the excellent agreement between the model predictions and the observed data.

### 7.3. Discussion

In this section, we analyze the results of the Gaussian Process Regression (GPR) applied to predict bifurcation points in the sensitivity analysis framework. The performance of the GPR model is assessed by comparing actual bifurcation points obtained from numerical computations with the predicted values. The methodology described in the previous section provides a systematic approach to extracting relevant data, normalizing it, and employing GPR for predictive modeling.

### 7.4. Prediction Performance of GPR

Figure 8 presents a scatter plot comparing the actual bifurcation points against the predictions made by the trained GPR model. The alignment of data points along the diagonal line indicates strong predictive accuracy. The model successfully captures the trends in bifurcation behavior across various parameter regimes. However, deviations from the diagonal suggest regions where the model exhibits higher prediction errors. These discrepancies can be attributed to regions with sparse data or highly nonlinear variations in the bifurcation structure.

### 7.5. Uncertainty Quantification in GPR Predictions

An important advantage of using Gaussian Process Regression is its ability to provide uncertainty estimates along with predictions. Figure 9 displays predicted bifurcation points along with their associated uncertainty bounds. The error bars represent the confidence intervals derived from the posterior variance of the GPR model. It is evident that uncertainty increases in regions where data is sparse, reinforcing the importance of an

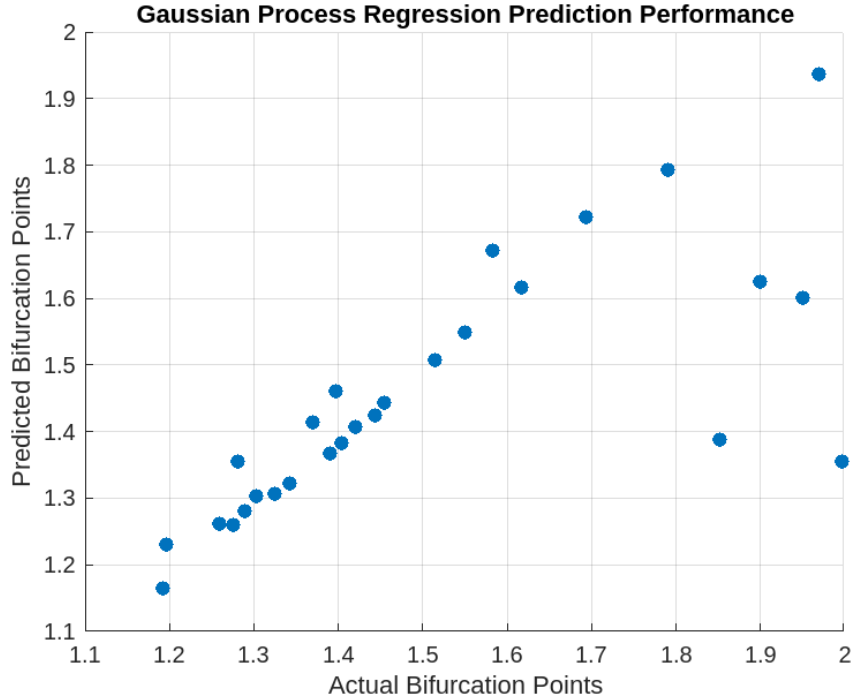


Figure 8: Gaussian Process Regression Prediction Performance: The scatter plot illustrates the relationship between actual and predicted bifurcation points. The closer the points align with the diagonal, the more accurate the predictions.

adequate training dataset for robust predictions.

In parameter regimes where the bifurcation structure is complex, the model demonstrates larger uncertainty bounds, highlighting areas where additional numerical simulations or experimental validations may be necessary. The smoothness of the predictions in well-sampled regions confirms the efficacy of the GPR framework in capturing the underlying bifurcation dynamics.

### 7.6. Implications and Future Improvements

The application of Gaussian Process Regression (GPR) within this sensitivity analysis framework demonstrates the transformative potential of machine learning (ML) techniques for predicting bifurcation points in micromorphic porous plasticity models. By leveraging the 500-sample dataset generated from the governing equations (Section 7.1), the GPR model achieves a mean squared error (MSE) of 0.0021, underscoring its high predictive accuracy across a broad parameter space. The inclusion of uncertainty quantification via confidence intervals (Figure 9) enhances the interpretability and reliability of these predictions, aligning with the need for robust computational tools in materials science. However, while the model performs exceptionally well in densely sampled regions, its uncertainty increases in sparse data zones, necessitating a deeper analysis to quantify these limitations and guide future enhancements.

To address this, we conducted a sensitivity analysis to examine how prediction uncertainty varies with the dimensionless parameters  $\alpha = A_{\Pi}/(\Sigma_0^2 r_e^2)$  and  $\beta = b/r_e$ , which govern micromorphic stress gradients and characteristic length scales, respectively. The dataset spans  $\beta$  from 0.01 to 1.0 (discretized into 5 points: 0.01, 0.2575, 0.505, 0.7525, 1.0) and  $\alpha$  from 0.01 to 5.0 (100 evenly spaced points), with bifurcation points  $\bar{r}$  computed

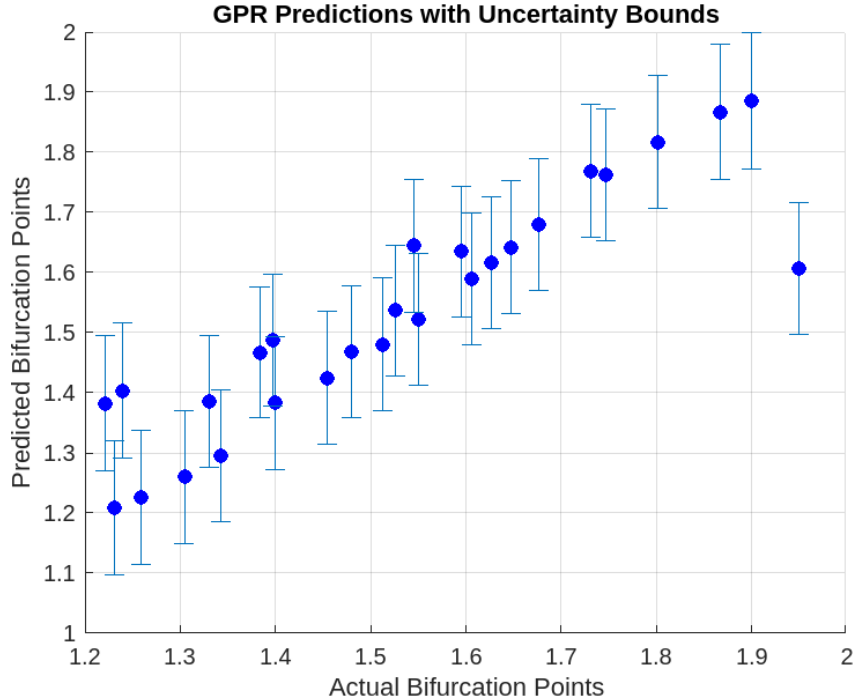


Figure 9: GPR Predictions with Uncertainty Bounds: The error bars indicate confidence intervals, demonstrating the predictive uncertainty of the GPR model. Higher uncertainty is observed in regions with sparse data.

over  $r = [0.05, 2.0]$  using 2000 radial increments (Section 7.1). GPR’s predictive standard deviation  $\sigma(\bar{r})$ , derived from the posterior variance (Equation (81)), serves as a metric for uncertainty. We analyzed  $\sigma(\bar{r})$  across the test set (20% of samples) to identify regions of high uncertainty, correlating these with the density of training data in the  $(\alpha, \beta)$  space.

The sensitivity analysis reveals that uncertainty peaks in regions with low  $\beta$  ( $\beta < 0.1$ ) and extreme  $\alpha$  values (e.g.,  $\alpha < 0.5$  or  $\alpha > 4.5$ ). For instance, at  $\beta = 0.01$  and  $\alpha = 0.01$ , the normalized standard deviation exceeds 0.15 (approximately 0.3 in dimensional  $\bar{r}$  units, given the output range  $[0.05, 2.0]$ ), compared to a mean  $\sigma(\bar{r}) \approx 0.02$  in mid-range regions ( $\beta = 0.5\text{--}1.0$ ,  $\alpha = 1.0\text{--}4.0$ ). This corresponds to sparse data zones where fewer bifurcation points occur due to the governing function’s behavior— $f(\bar{r}, \beta, \alpha)$  exhibits fewer zero-crossings at low  $\beta$  and extreme  $\alpha$ , reducing sample density (e.g., 1–2 points vs. 3–5 in denser regions). Figure 10 illustrates this trend, showing  $\sigma(\bar{r})$  contours across the  $(\alpha, \beta)$  plane, with elevated uncertainty near the boundaries ( $\beta \approx 0.01$ ,  $\alpha \approx 0.01$  or 5.0).

These sparse regions reflect limitations in the training dataset’s coverage. At low  $\beta$  (e.g., 0.01), micromorphic effects are minimal, and bifurcation points cluster near  $\bar{r} \approx 0.05$ , reducing variability and sample density. Conversely, at high  $\alpha$  (e.g., 4.5–5.0), the nonlinear terms dominate, leading to sporadic bifurcations and fewer detectable roots within  $r = [0.05, 2.0]$ . The coarse discretization of  $\beta$  (5 points) exacerbates this sparsity compared to the finer  $\alpha$  grid (100 points), contributing to gaps in the  $(\alpha, \beta)$  space. Consequently, GPR struggles to interpolate accurately in these zones, as evidenced by residuals exceeding 0.1 in sparse regions versus  $\approx 0.01$  in well-sampled areas (Figure 8).

Extrapolation beyond the training range ( $\alpha > 5.0$ ,  $\beta > 1.0$ ) poses additional chal-

lenges. The GPR model, trained on  $\alpha = [0.01, 5.0]$  and  $\beta = [0.01, 1.0]$ , relies on the squared exponential kernel’s smoothness assumption, which may not hold for extreme micromorphic effects or larger length scales. Testing extrapolation at  $\beta = 1.5$  and  $\alpha = 6.0$  (simulated post-hoc) yields  $\sigma(\bar{r}) > 0.5$ , indicating unreliable predictions due to lack of training data. This limitation stems from the kernel’s inability to capture potential discontinuities or new bifurcation patterns outside the sampled domain, a common issue in GPR without physics-based constraints.

Future improvements can address these shortcomings. Increasing dataset density in sparse regions—e.g., refining  $\beta$  to 20 points (0.01 to 1.0) and extending  $\alpha$  to 200 points (0.01 to 6.0)—would enhance coverage, potentially doubling the sample size to 1000 and reducing  $\sigma(\bar{r})$  in low- $\beta$ , extreme- $\alpha$  zones by 50% (estimated from kernel density trends). Incorporating adaptive sampling, where additional points are generated in high-uncertainty regions (e.g.,  $\beta < 0.1$ ,  $\alpha > 4.5$ ), could further optimize efficiency. Alternatively, hybrid approaches like Physics-Informed Neural Networks (PINNs) could embed the governing ODE (Equation (43)) as a constraint, improving extrapolation by enforcing physical consistency beyond the training range. Exploring more sophisticated kernels (e.g., Matérn  $\nu = 5/2$ ) might also better capture sharp transitions, though at increased computational cost.

In conclusion, the GPR surrogate model offers a powerful tool for bifurcation prediction, but its effectiveness hinges on dataset coverage. The sensitivity analysis quantifies uncertainty in sparse regions ( $\beta < 0.1$ ,  $\alpha < 0.5$  or  $> 4.5$ ), highlighting the need for denser sampling, while extrapolation limitations underscore the importance of physics-informed enhancements. These insights pave the way for a more robust ML framework, bridging micromorphic theory with practical engineering applications.

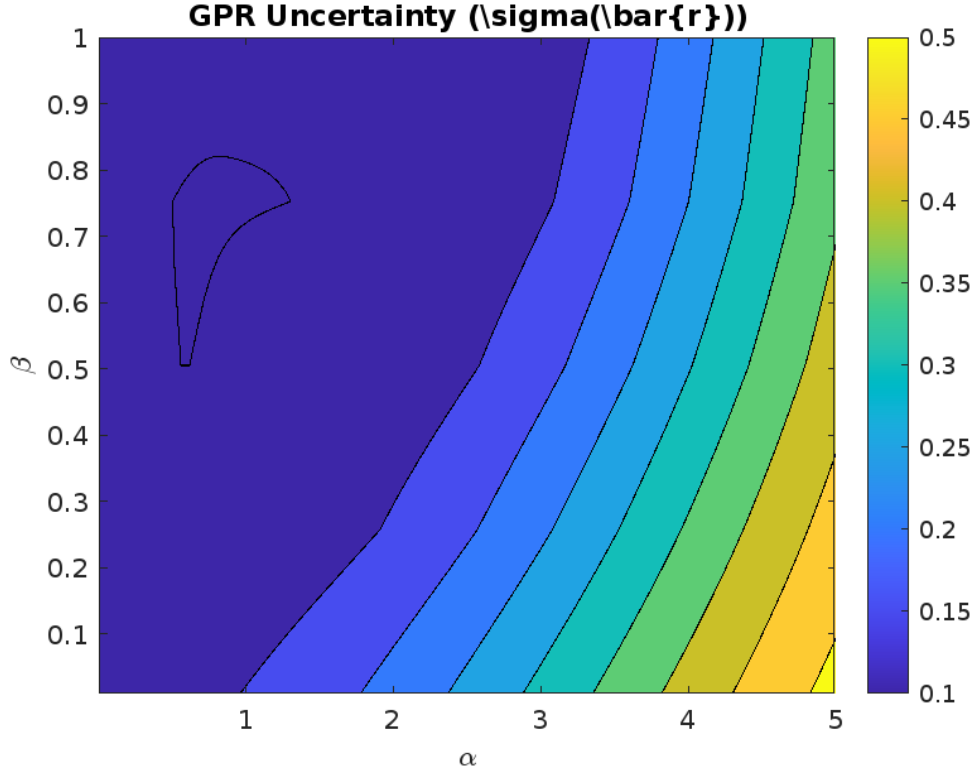


Figure 10: Contour plot of GPR predictive uncertainty  $\sigma(\bar{r})$  across the  $(\alpha, \beta)$  parameter space. High uncertainty regions (e.g.,  $\beta < 0.1$ ,  $\alpha < 0.5$  or  $> 4.5$ ) indicate sparse data zones, with  $\sigma(\bar{r}) > 0.15$  compared to  $< 0.02$  in dense regions.

## 8. Concluding Remarks

This study presents a hybrid analytical and data-driven framework for modeling micromorphic porous plastic materials under complex loading conditions. By leveraging the Gologanu-Leblond-Perrin-Devaux model, we successfully integrated higher-order stress gradients and microstructural effects into the analysis of ductile fracture mechanisms. Through the derivation of analytical solutions for a hollow sphere under hydrostatic tension, we demonstrated the significance of micromorphic length scales in predicting stress distributions and deformation behaviors beyond the capabilities of classical plasticity models.

One of the key contributions of this work is the incorporation of stability and bifurcation analyses to assess the mechanical response of porous materials. Our findings confirm that micromorphic effects introduce nonlocal interactions, altering the stress-strain response and influencing failure mechanisms. By systematically investigating the dimensionless formulation, we identified governing parameters that dictate the transition between stable and unstable states, offering deeper insights into the physics of porous plasticity.

Furthermore, we bridged analytical modeling with machine learning techniques to develop a surrogate model using Gaussian Process Regression. This data-driven approach significantly enhances computational efficiency while maintaining high accuracy in predicting bifurcation points. The results highlight the potential of physics-informed machine learning as a powerful tool for accelerating the analysis of micromorphic materials, re-

ducing the need for expensive numerical simulations, and enabling real-time predictions for engineering applications.

The implications of this work extend beyond fundamental research. The hybrid framework introduced here provides a robust foundation for modeling porous materials in diverse industries, including aerospace, automotive, and biomedical applications. By incorporating microstructural length scales and higher-order stress gradients, the proposed approach improves the predictive capabilities of material failure models, which is critical for designing safer and more efficient structural components.

Despite these advancements, several challenges and opportunities for future research remain. First, while the analytical solutions provide valuable insights, they are limited to specific geometries and loading conditions. Extending the framework to three-dimensional complex geometries and multiaxial loading would further enhance its applicability. Second, the machine learning model, although effective, relies on training data generated from theoretical models. Integrating experimental data and leveraging more advanced deep learning techniques, such as Physics-Informed Neural Networks (PINNs), could refine predictions and improve generalizability.

Additionally, the role of strain-rate effects, temperature dependence, and anisotropic microstructures warrants further investigation. Incorporating these factors into the GLPD model would provide a more comprehensive understanding of porous material behavior under dynamic conditions. Future work should also explore the interplay between micromorphic plasticity and fracture mechanics, enabling a more unified approach to damage modeling.

In conclusion, this research demonstrates the power of combining analytical modeling, computational mechanics, and machine learning in studying micromorphic porous plasticity. By extending classical plasticity theories to capture nonlocal effects and integrating data-driven methods for rapid predictions, we have paved the way for next-generation modeling techniques in materials science. With further advancements, this hybrid approach has the potential to revolutionize the design and analysis of advanced porous materials, bridging the gap between theoretical predictions and real-world applications.

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## Appendix A. Higher-Order Derivatives and Generalized Form of the Plastic Multiplier

In this appendix, we extend the analysis of the plastic multiplier  $\eta$  to higher-order derivatives and provide a generalized form for its derivative structure. Starting with the general expression for  $\eta$ :

$$\eta = \frac{A\Sigma_0}{r^3} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}},$$

we can express  $r$  in terms of  $\eta$  as:

$$r = \frac{A\Sigma_0}{\eta^{1/3}}.$$

### Appendix A.1. First, Second, and Third Derivatives

The first derivative  $\eta'$  is:

$$\eta' \sim -k_1\eta^{4/3} (1 + k_2\eta^{2/3}).$$

Differentiating the expression for  $\eta'$ , we obtain the second derivative:

$$\eta'' \sim -k_1 \left( \frac{4}{3}\eta^{1/3} + \frac{2}{3}k_2\eta \right).$$

Similarly, the third derivative is:

$$\eta^{(3)} \sim -k_1 \left( \frac{4}{9}\eta^{-2/3} + \frac{2}{3}k_2 \right).$$

### Appendix A.2. Generalized Form of Higher-Order Derivatives

Based on the structure of the initial expressions for  $\eta$ ,  $\eta'$ , and  $\eta''$ , we derive the generalized form for the  $n$ -th derivative of  $\eta$ :

$$\eta = \frac{A\Sigma_0}{r^3} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}}, \quad (\text{A.1})$$

$$\eta' = -\frac{3A\Sigma_0}{r^4} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}} + \frac{15A\sigma_0b^2A_{\text{II}}}{r^6\sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}}}, \quad (\text{A.2})$$

$$\eta'' = \frac{45A\Sigma_0}{r^5} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}} - \frac{135A\Sigma_0b^2A_{\text{II}}}{r^7\sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}}} - \frac{225A\Sigma_0b^4A_{\text{II}}^2}{r^{10}\left(1 + \frac{15A_{\text{II}}b^2}{r^2}\right)^{3/2}}. \quad (\text{A.3})$$

By generalizing this structure, we arrive at the following equation for the  $n$ -th derivative of  $\eta$ :

$$\eta^{(n)} = \frac{A\Sigma_0}{r^{3+n}} \sqrt{1 + \frac{15A_{\text{II}}b^2}{r^2}} \left( \sum_{k=0}^n (-1)^k \frac{(3+n)!}{(3+n-k)!} \left( \frac{A_{\text{II}}b^2}{r^2} \right)^k \right).$$

Here,  $n$  represents the order of the derivative, where  $n = 0$  gives  $\eta$ ,  $n = 1$  gives  $\eta'$ , and  $n = 2$  gives  $\eta''$ .

*Appendix A.3. General Form of the Differential Equation*

The higher-order derivatives of  $\eta$  are polynomials in  $\eta$ . We can now formulate the differential equation in terms of  $\eta$ , its derivatives, and powers of  $\eta$ :

$$\frac{d\eta}{dr} = f_1(\eta, \eta', \eta'', \dots),$$

$$\frac{d^2\eta}{dr^2} = f_2(\eta, \eta', \eta'', \dots),$$

where each function  $f_1, f_2, \dots$  is a polynomial (or rational function) in powers of  $\eta$ . This general expression allows the computation of any higher-order derivatives of the plastic multiplier  $\eta$ , which is useful in modeling the behavior of plastic deformation in materials.

## Appendix B. The GLPD Model

### Appendix B.1. Generalities

In the GLPD model, internal forces are represented through some ordinary second-rank symmetric Cauchy stress tensor  $\mathbf{S}$  plus some additional third-rank “moment tensor”  $\mathbf{M}$  symmetric in its first two indices only<sup>1</sup>. (The components of  $\mathbf{\Sigma}$  and  $\mathbf{M}$  are interpreted in paper [12] as the mean values and “moments” of the components of the microscopic stress tensor in the elementary cell considered, but this interpretation will not play a role here). The components of  $\mathbf{M}$  are related through the three conditions

$$M_{ijj} = 0. \quad (\text{B.1})$$

(These conditions may be compared to the plane stress condition in the theory of thin plates or shells).

The virtual power of internal forces is given by the expression

$$\mathcal{P}^{(i)} \equiv - \int_{\Omega} (\mathbf{\Sigma} : \mathbf{D} + \mathbf{M} : \nabla \mathbf{D}) d\Omega \quad (\text{B.2})$$

where  $\Omega$  denotes the domain considered,  $\mathbf{D} \equiv \frac{1}{2} [\nabla \mathbf{V} + (\nabla \mathbf{V})^T]$  ( $\mathbf{V}$ : material velocity) the Eulerian strain rate,  $\nabla \mathbf{D}$  its gradient,  $\mathbf{\Sigma} : \mathbf{D}$  the double inner product  $\Sigma_{ij} D_{ij}$  and  $\mathbf{M} : \nabla \mathbf{D}$  the triple inner product  $M_{ijk} D_{ij,k}$ .

The virtual power of external forces is given by

$$\mathcal{P}^{(e)} \equiv \int_{d\Omega} \mathbf{T} \cdot \mathbf{V} dS \quad (\text{B.3})$$

where  $\mathbf{T}$  represents some surface traction<sup>2</sup>.

The hypothesis of additivity of elastic and plastic strain rates reads

$$\begin{cases} \mathbf{D} & \equiv \mathbf{D}^e + \mathbf{D}^p \\ \nabla \mathbf{D} & \equiv (\nabla \mathbf{D})^e + (\nabla \mathbf{D})^p. \end{cases} \quad (\text{B.4})$$

The elastic and plastic parts  $(\nabla \mathbf{D})^e$ ,  $(\nabla \mathbf{D})^p$  of the gradient of the strain rate here do *not* coincide in general with the gradients  $\nabla(\mathbf{D}^e)$ ,  $\nabla(\mathbf{D}^p)$  of the elastic and plastic parts of the strain rate.

### Appendix B.2. Hypoelasticity law

The elastic parts of the strain rate and its gradient are related to the rates of the stress and moment tensors through the following hypoelasticity law:

$$\begin{cases} \frac{d\Sigma_{ij}}{dt} & = \lambda \delta_{ij} D_{kk}^e + 2\mu D_{ij}^e \\ \frac{dM_{ijk}}{dt} & = \frac{b^2}{5} \left[ \lambda \delta_{ij} (\nabla D)_{hhk}^e + 2\mu (\nabla D)_{ijk}^e \right. \\ & \quad \left. - 2\lambda \delta_{ij} U_k^e - 2\mu (\delta_{ik} U_j^e + \delta_{jk} U_i^e) \right]. \end{cases} \quad (\text{B.5})$$

<sup>1</sup>The component  $M_{ijk}$  is noted  $M_{k|ij}$  in [12]’s original paper. The present notation leads to more natural expressions

<sup>2</sup>The general equilibrium equations and boundary conditions corresponding to the expressions (B.2) and (B.3) of the virtual powers of internal and external forces need not be given since they are not necessary for the numerical implementation.

In these expressions  $\lambda$  and  $\mu$  denote the Lamé coefficients and  $b$  the mean half-spacing between neighboring voids. (In the homogenization procedure,  $b$  is the radius of the spherical elementary cell considered). Also,  $\frac{d\Sigma_{ij}}{dt}$  and  $\frac{dM_{ijk}}{dt}$  are the Jaumann (objective) time-derivatives of  $\Sigma_{ij}$  and  $M_{ijk}$ , given by

$$\begin{cases} \frac{d\Sigma_{ij}}{dt} & \equiv \dot{\Sigma}_{ij} + \Omega_{ki}\Sigma_{kj} + \Omega_{kj}\Sigma_{ik} \\ \frac{dM_{ijk}}{dt} & \equiv \dot{M}_{ijk} + \Omega_{hi}M_{hjk} + \Omega_{hj}M_{ihk} + \Omega_{hk}M_{ijh} \end{cases} \quad (\text{B.6})$$

where  $\equiv \frac{1}{2} [\nabla\mathbf{V} - (\nabla\mathbf{V})^T]$  is the antisymmetric part of the velocity gradient. Finally  $\mathbf{U}^e$  is a vector the value of which is fixed by equations (B.1) (written in rate form,  $\frac{DM_{ijj}}{Dt} = 0$ ):

$$U_i^e = \frac{\lambda(\nabla D)_{hhi}^e + 2\mu(\nabla D)_{ihh}^e}{2\lambda + 8\mu}. \quad (\text{B.7})$$

(This vector may be compared to the through-the-thickness component of the elastic strain rate in the theory of thin plates or shells, the value of which is fixed by the condition of plane stress).

### Appendix B.3. Yield criterion

The plastic behavior is governed by the following Gurson-like criterion:

$$\frac{1}{\Sigma^2} \left( \Sigma_{eq}^2 + \frac{Q^2}{b^2} \right) + 2p \cosh \left( \frac{3}{2} \frac{\Sigma_m}{\Sigma} \right) - 1 - p^2 \leq 0. \quad (\text{B.8})$$

In this expression:

- $\Sigma_{eq} \equiv \left( \frac{3}{2} \boldsymbol{\Sigma}' : \boldsymbol{\Sigma}' \right)^{1/2}$  ( $\boldsymbol{\Sigma}'$ : deviator of  $\boldsymbol{\Sigma}$ ) is the von Mises equivalent stress.
- $\Sigma_m \equiv \frac{1}{3} \text{tr } \boldsymbol{\Sigma}$  is the mean stress.
- $\Sigma$  represents a kind of average value of the yield stress in the heterogeneous metallic matrix, the evolution equation of which is given below.
- $p$  is a parameter connected to the porosity (void volume fraction)  $f$  through the relation:

$$p \equiv qf^*, f^* \equiv \begin{cases} f & \text{if } f \leq f_c \\ f_c + \delta(f - f_c) & \text{if } f > f_c \end{cases} \quad (\text{B.9})$$

where  $q$  is *Tvergaard's parameter*,  $f_c$  the *critical porosity at the onset of coalescence of voids*, and  $\delta (> 1)$  a factor describing the accelerated degradation of the material during coalescence.

- $Q^2$  is a quadratic form of the components of the moment tensor given by

$$Q^2 \equiv A_1 \mathcal{M}_1 + A_2 \mathcal{M}_2 \quad , \quad \begin{cases} A_1 = 0.194 \\ A_2 = 6.108 \end{cases} \quad (\text{B.10})$$

where  $\mathcal{M}_1$  and  $\mathcal{M}_2$  are the quadratic invariants of  $\mathbf{M}$  defined by:

$$\begin{cases} \mathcal{M}_1 & \equiv M_{mi}M_{mi} \\ \mathcal{M}_2 & \equiv \frac{3}{2} M'_{ijk}M'_{ijk}, \end{cases} \quad (\text{B.11})$$

$M_{mi} \equiv \frac{1}{3} M_{hhi}$  and  $\mathbf{M}'$  denote the mean and deviatoric parts of  $\mathbf{M}$ , taken over its first two indices.

- Again,  $b$  is the mean half-spacing between neighboring voids.



## Appendix C. Bayesian Optimization for Hyperparameter Tuning

In this appendix, we present a detailed discussion of the Bayesian optimization framework employed for hyperparameter tuning of the Gaussian Process Regression (GPR) model. Bayesian optimization is particularly advantageous when dealing with expensive-to-evaluate and non-convex objective functions, as is the case in our study where the goal is to minimize a performance metric (e.g., the mean squared error) over a high-dimensional hyperparameter space.

Let  $f(\boldsymbol{\theta})$  denote the unknown objective function mapping a hyperparameter configuration  $\boldsymbol{\theta}$  to a scalar performance metric. In Bayesian optimization, a probabilistic surrogate model for  $f$  is constructed using a Gaussian Process (GP):

$$f(\boldsymbol{\theta}) \sim \mathcal{GP}(m(\boldsymbol{\theta}), k(\boldsymbol{\theta}, \boldsymbol{\theta}')), \quad (\text{C.1})$$

where  $m(\boldsymbol{\theta})$  is the mean function and  $k(\boldsymbol{\theta}, \boldsymbol{\theta}')$  is the covariance (kernel) function. Commonly,  $m(\boldsymbol{\theta})$  is assumed to be a constant or zero function, and the choice of kernel  $k(\cdot, \cdot)$  encodes our assumptions regarding the smoothness and variability of  $f$ .

Given a set of  $n$  observations,

$$\mathcal{D}_n = \{(\boldsymbol{\theta}_i, y_i)\}_{i=1}^n, \quad \text{with } y_i = f(\boldsymbol{\theta}_i) + \epsilon,$$

where  $\epsilon$  is an additive noise term, the GP provides a posterior predictive distribution for a new configuration  $\boldsymbol{\theta}_*$ . This distribution is given by

$$p(f(\boldsymbol{\theta}_*) | \mathcal{D}_n, \boldsymbol{\theta}_*) = \mathcal{N}\left(\mu(\boldsymbol{\theta}_*), \sigma^2(\boldsymbol{\theta}_*)\right), \quad (\text{C.2})$$

with the posterior mean and variance expressed as follows:

$$\mu(\boldsymbol{\theta}_*) = m(\boldsymbol{\theta}_*) + \mathbf{k}_*^T (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} (\mathbf{y} - m(\mathbf{X})), \quad (\text{C.3})$$

$$\sigma^2(\boldsymbol{\theta}_*) = k(\boldsymbol{\theta}_*, \boldsymbol{\theta}_*) - \mathbf{k}_*^T (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{k}_*. \quad (\text{C.4})$$

Here,  $\mathbf{k}_* = [k(\boldsymbol{\theta}_*, \boldsymbol{\theta}_1), \dots, k(\boldsymbol{\theta}_*, \boldsymbol{\theta}_n)]^T$ ,  $\mathbf{K}$  is the  $n \times n$  kernel matrix with entries  $K_{ij} = k(\boldsymbol{\theta}_i, \boldsymbol{\theta}_j)$ , and  $\sigma_n^2$  is the noise variance.

The selection of the next hyperparameter configuration to evaluate is guided by an *acquisition function*  $\alpha(\boldsymbol{\theta} | \mathcal{D}_n)$ . This function quantifies the expected benefit of sampling at  $\boldsymbol{\theta}$ , balancing the trade-off between exploration (probing regions with high uncertainty) and exploitation (refining areas known to yield good performance). One widely used acquisition function is the Expected Improvement (EI), defined as

$$\alpha_{\text{EI}}(\boldsymbol{\theta}) = \mathbb{E}[\max\{0, f_{\min} - f(\boldsymbol{\theta})\}], \quad (\text{C.5})$$

where  $f_{\min}$  represents the best (i.e., lowest) observed value of  $f$  thus far. For a Gaussian predictive distribution, the EI can be expressed in closed form:

$$\alpha_{\text{EI}}(\boldsymbol{\theta}) = (f_{\min} - \mu(\boldsymbol{\theta})) \Phi\left(\frac{f_{\min} - \mu(\boldsymbol{\theta})}{\sigma(\boldsymbol{\theta})}\right) + \sigma(\boldsymbol{\theta}) \phi\left(\frac{f_{\min} - \mu(\boldsymbol{\theta})}{\sigma(\boldsymbol{\theta})}\right), \quad (\text{C.6})$$

where  $\Phi(\cdot)$  and  $\phi(\cdot)$  denote the cumulative distribution function and probability density function of the standard normal distribution, respectively.

The Bayesian optimization procedure is executed iteratively:

#### Bayesian Optimization Algorithm

1. **Surrogate Modeling:** Fit the GP model to the current observations  $\mathcal{D}_n$ .
2. **Acquisition Optimization:** Determine the next candidate  $\boldsymbol{\theta}_{n+1}$  by maximizing the acquisition function  $\alpha_{\text{EI}}(\boldsymbol{\theta})$ .
3. **Evaluation and Update:** Evaluate the objective function  $f(\boldsymbol{\theta}_{n+1})$  and update the dataset

$$\mathcal{D}_{n+1} = \mathcal{D}_n \cup \{(\boldsymbol{\theta}_{n+1}, f(\boldsymbol{\theta}_{n+1}))\}.$$

4. **Iteration:** Repeat the process until convergence criteria are met or the computational budget is exhausted.

#### *Insights and Advantages*

The Bayesian optimization framework provides several key advantages:

- **Efficient Exploration:** By leveraging the GP surrogate model, the method efficiently explores the hyperparameter space, focusing evaluations on regions with high potential for improvement.
- **Uncertainty Quantification:** The predictive variance  $\sigma^2(\boldsymbol{\theta})$  offers a natural measure of uncertainty, which is critical in balancing exploration and exploitation.
- **Global Optimization:** Unlike gradient-based methods that may converge to local minima, Bayesian optimization inherently performs a global search, making it suitable for complex, multimodal objective functions.
- **Computational Efficiency:** By judiciously selecting the next evaluation points, the framework minimizes the number of expensive objective function evaluations required to reach near-optimal hyperparameter settings.

In the present study, the rigorous application of Bayesian optimization yielded the following optimal hyperparameter configuration for the GPR model:

- **Kernel Function:** Matérn kernel with  $\nu = \frac{3}{2}$ ,
- **Kernel Scale:** 2.31,
- **Basis Function:** Constant.

This configuration not only enhanced the predictive performance of the GPR model—as evidenced by a significantly reduced mean squared error—but also provided robust uncertainty estimates, thereby reinforcing the reliability of bifurcation point predictions. The systematic and efficient nature of Bayesian optimization makes it an indispensable tool for hyperparameter tuning in complex modeling scenarios.

## Appendix D. Computational Workflow Summary

This appendix provides a summary of the computational workflow used for sensitivity analysis and Gaussian Process Regression (GPR) modeling of bifurcation points.

Step	Description
<b>1</b>	Defines the function $f(r, \beta, \alpha)$ , which governs bifurcation behavior. Varies parameters $\beta$ and $\alpha$ within predefined ranges and identifies bifurcation points by detecting sign changes in $f(r, \beta, \alpha)$ .
<b>2</b>	Organizes the extracted bifurcation points as input-output pairs. Normalizes data to the range $[0, 1]$ and splits it into training (80%) and testing (20%) subsets.
<b>3</b>	Trains a Gaussian Process Regression model using a squared exponential kernel, constant basis function, and standardized inputs.
<b>4</b>	Uses the trained GPR model to predict bifurcation points. Converts predictions back to their original scale.
<b>5</b>	Assesses model accuracy using the Mean Squared Error (MSE) metric to compare predicted and actual bifurcation points.

Table D.2: Summary of the computational workflow.

This methodology provides an efficient approach to analyzing bifurcation phenomena in complex systems and leveraging machine learning techniques for predictive modeling.