

**EFFICIENT NUMERICAL SCHEMES FOR FINITE DEFORMATION
PLASTICITY: KINEMATIC HARDENING, MULTI-INVARIANTS
DEPENDENCE AND PHASE FIELD COUPLING**

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**Efficient Numerical Schemes for Finite Deformation Plasticity:
Kinematic Hardening, Multi-invariants Dependence and Phase Field
Coupling**

by

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*Dedicated to
my mother*

CERTIFICATE

This is to certify that the thesis entitled “**Efficient Numerical Schemes for Finite Deformation Plasticity: Kinematic Hardening, Multi-invariants Dependence and Phase Field Coupling**” being submitted by **Mr. Sumit Kumar** to the Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy** in Applied Mechanics is a record of original, bonafide record of research work carried out by him under my supervision and guidance. The thesis work, in my opinion, has reached the requisite standard, fulfilling the requirements for the degree of Doctor of Philosophy.

The results contained in this thesis have not been submitted, in part or in full, to any other university or institute for the award of any degree or diploma.

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Abstract

Plasticity plays an important role in the manufacturing, design, and failure investigation of components/structures made up of metallic materials. Such components may be subjected to a complex state of stress and may undergo finite deformation under monotonic/cyclic loading. Based on the literature review, it is found that the covariant formulation of nonlinear kinematic hardening, the effects of stress triaxiality, and Lode parameters on ductile response/failure, viscoplasticity, and their coupling with phase field theory are not adequately dealt with. In the present thesis, isotropic plasticity is investigated by considering nonlinear kinematic hardening, multi-invariants dependence, and viscoplasticity with coupling to phase field theory for small and large deformations, along with the examination of numerical implementation aspects.

A covariant formulation of hyperelasto-plasticity, including the nonlinear kinematic hardening, is presented in finite deformation plasticity. A nonlinear kinematic hardening equation is proposed in the spatial configuration using the Lie derivative of the kinematic hardening tensor. A method is proposed to compute the deviatoric and trace parts of the elastic left Cauchy Green tensor and the deviatoric part of the kinematic hardening tensor, satisfying the incompressibility of plastic deformation. The integration of the local governing equations using the covariant backward Euler integration scheme is presented along with the closed-form expression of the algorithmically consistent spatial tangent constitutive tensor.

A ductile failure theory is presented by coupling the developed covariant formulation of kinematic hardening finite deformation plasticity with phase field theory. To capture the correct physical response of the material after crack initiation, the fracture driving function is modified by an energy release controlling function. A neural network optimization procedure is presented to calibrate the material parameters. The capability of the model is demonstrated by simulating the crack path in complex three-dimensional geometries.

Implicit and semi-implicit integration schemes are formulated for multi-invariants dependent finite deformation plasticity. In the implicit integration scheme, the backward Euler difference approximation

of equivalent plastic strain is coupled with the exponential approximation of return mapping in principal Kirchhoff stresses space. In the semi-implicit integration scheme, the forward Euler difference approximation of equivalent plastic strain is coupled with the logarithmic approximation of return mapping in Kirchhoff stress space. The computation time involved in the simulations using these two schemes is compared.

The multi-invariants dependent plasticity is coupled with phase field theory to investigate the effects of stress invariants on crack initiation and propagation in ductile materials. The threshold energy in the phase field variable evolution equation is proposed as a function of the stress triaxiality and normalized Lode angle parameters based on the Mohr-Coulomb fracture initiation criterion. A Hosford equivalent stress-dependent Drucker-Prager yield function is used to describe the ductile response of the material, which provides stress invariants dependent energy release during the crack propagation. The experimental responses of different specimens with varying degrees of stress triaxiality and Lode angle parameters available in the literature are used to calibrate model parameters. The simulated crack propagation path in these specimens is compared with that observed in available experimental studies.

To consider the rate-dependent behavior of materials, an accurate and computationally efficient integration scheme is proposed for small deformation viscoplasticity by combining the backward Euler difference approximation of the stress rate equation and the exponential integration scheme for the kinematic hardening equation. The accuracy and computational cost of the proposed integration scheme are compared with the integration schemes based on either backward Euler difference approximation or exponential integration. Finally, a preliminary study involving small deformation viscoplasticity coupled with phase field theory is carried out to investigate low cycle fatigue and creep interaction.

सारांश

प्लास्टिसिटी धातुयुक्त पदार्थों/संरचनाओं के निर्माण, डिजाइन, और विफलता जांच में महत्वपूर्ण भूमिका निभाती है। इस प्रकार के घटक मोनोटोनिक/साइक्लिक लोडिंग के तहत जटिल प्रतिबल तथा सीमित विकृति की अवस्था में हो सकते हैं। साहित्य की समीक्षा के आधार पर यह पाया गया है कि सहसंयोजक सूत्रीकरण का अरेखीय गतिकी कठोरीकरण, प्रतिबल त्रिअक्षीयता और लोड मापदण्डों का तन्व्य प्रतिक्रिया/विफलता पर प्रभाव, विस्कोप्लास्टी और इनके चरण क्षेत्र सिद्धांत के साथ युग्मन का पूर्णरूपेण अध्ययन नहीं किया गया है। वर्तमान शोध-ग्रंथ में, समदैशिक प्लास्टिसिटी का अध्ययन अरेखीय गतिकी कठोरीकरण, बहु-अपरिवर्तनीय (मल्टी-इन्वेरीअन्ट) पर निर्भरता, और विस्कोप्लास्टिसिटी का चरण क्षेत्र के साथ युग्मन के साथ कम तथा अधिक विकृतियों के लिए संख्यात्मक परीक्षण के साथ-साथ किया गया है।

हाइपरइलास्टो-प्लास्टिसिटी का एक सहसंयोजक सूत्रीकरण, जिसमें अरेखीय गतिकी कठोरीकरण भी शामिल है, परिमित विरूपण प्लास्टिसिटी में प्रस्तुत किया गया है। गतिज कठोरीकरण टेंसर के ली व्युत्पन्न का उपयोग करके स्थानिक विन्यास में एक अरेखीय गतिज कठोरीकरण समीकरण प्रस्तावित किया गया है। प्लास्टिक विरूपण की असंपीड्यता को संतुष्ट करते हुए, प्रत्यास्थ बाएं कॉची ग्रीन टेंसर के विचलन और ट्रेस भागों और गतिज कठोरीकरण टेंसर के विचलन भाग की गणना करने के लिए एक विधि प्रस्तावित की गयी है। सहसंयोजक पश्चवर्ती यूलर समाकलन विधि का उपयोग करके स्थानीय गवर्निंग समीकरणों के समाकलन को एल्गोरिदमिक रूप से सुसंगत स्थानिक स्पष्टरेखा कोंस्टीट्यूटिव टेंसर की क्लोज्ड फॉर्म अभिव्यक्ति के साथ प्रस्तुत किया गया है।

चरण क्षेत्र सिद्धांत के साथ गतिकी सख्त परिमित विरूपण प्लास्टिसिटी के विकसित किये गये सहसंयोजक सूत्रीकरण को युग्मित करके एक तन्व्य विफलता सिद्धांत प्रस्तुत किया गया है। दरार शुरू होने के बाद पदार्थ की सही भौतिक प्रक्रिया को पकड़ने के लिए, फ्रैक्चर ड्राइविंग फ्रंक्शन को ऊर्जा रिलीज नियंत्रण फ्रंक्शन द्वारा संशोधित किया गया है। पदार्थ गुण मापदंडों को ज्ञात करने के लिए एक तंत्रिका नेटवर्क अनुकूलन प्रक्रिया प्रस्तुत की गई है। जटिल त्रि-आयामी ज्यामिति में दरार पथ की सही गणना करके मॉडल की क्षमता प्रदर्शित की गयी है।

बहु-अपरिवर्तनीय पर निर्भर परिमित विरूपण प्लास्टिसिटी के लिए अंतर्निहित और अर्ध-अंतर्निहित समाकलन की योजनाएं ज्ञापित की गयी हैं। अंतर्निहित समाकलन योजना में, समतुल्य प्लास्टिक विकृति के पश्चवर्ती यूलर अंतर सन्निकटन को प्रिंसिपल किरचॉफ प्रतिबल स्पेस में रिटर्न मैपिंग के घातीय सन्निकटन के साथ प्रयोग किया गया है। अर्ध-अंतर्निहित समाकलन योजना में, समतुल्य प्लास्टिक विकृति के अग्रिम यूलर अंतर सन्निकटन को किरचॉफ स्ट्रेस स्पेस में रिटर्न मैपिंग के लॉगरिदमिक सन्निकटन के साथ प्रयोग किया गया है। इन दो योजनाओं का उपयोग करके सिमुलेशन में लगने वाले गणना समय की तुलना की गयी है।

तन्य पदार्थों में दरार की शुरुआत और प्रसार पर तनाव अपरिवर्तनीयों के प्रभावों का अध्ययन करने के लिए, बहु-अपरिवर्तनीय निर्भर प्लास्टिसिटी को चरण क्षेत्र सिद्धांत के साथ युग्मित किया गया है। चरण क्षेत्र परिवर्तनीय विकास समीकरण में श्रेयोल्ड ऊर्जा को मोहर-कूलम्ब फ्रैक्चर के आरम्भ के मानदंड के आधार पर प्रतिबल त्रिअक्षीयता और सामान्यीकृत लोड कोण मापदंडों के एक फ़ंक्शन के रूप में प्रस्तावित किया गया है। पदार्थ की तन्य प्रतिक्रिया का वर्णन करने के लिए एक होसफोर्ड समतुल्य प्रतिबल-निर्भर ड्रकर-प्रेगर फील्ड फ़ंक्शन का उपयोग किया गया है, जो दरार प्रसार के दौरान प्रतिबल अपरिवर्तनीय पर निर्भर ऊर्जा प्रदान करता है। साहित्य में उपलब्ध प्रतिबल त्रिअक्षीयता और लोड कोण मापदंडों की अलग-अलग डिग्री वाले विभिन्न नमूनों की प्रयोगात्मक प्रतिक्रियाओं का उपयोग मॉडल पैरामीट्रो को निकलने के लिए किया गया है। इन नमूनों में सिम्युलेटेड दरार प्रसार पथ की तुलना उपलब्ध प्रायोगिक अध्ययनों में देखे गए पथ से की गई है।

पदार्थों के दर-निर्भर भौतिकी व्यवहार का अध्ययन करने के लिए, प्रतिबल दर समीकरण के पश्चवर्ती यूलर अंतर सन्निकटन और गतिज सख्त समीकरण के लिए घातीय समाकलन योजना को मिलाकर छोटे विरूपण विस्कोप्लास्टी के लिए एक सटीक और कम्प्यूटेशनल रूप से कुशल समाकलन योजना प्रस्तावित की गयी है। प्रस्तावित समाकलन योजना की सटीकता और कम्प्यूटेशनल समय की तुलना पश्चवर्ती यूलर अंतर सन्निकटन या घातीय समाकलन पर आधारित समाकलन योजनाओं से की गयी है। अंततः, कम चक्र विभांति और क्रीप की अन्योन्यक्रिया की जांच के लिए चरण क्षेत्र सिद्धांत के साथ युग्मित करके छोटे विरूपण विस्कोप्लास्टिकिटी को शामिल करते हुए एक प्रारंभिक अध्ययन किया गया है।

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Nomenclature and Abbreviations

English Notations

$\mathbf{B}$	Reference configuration
$\mathbf{B}_t$	Spatial configuration
$\bar{\mathbf{B}}_t$	Intermediate configuration
$\mathbf{C}$	Right Cauchy Green tensor
$\bar{\mathbf{C}}^e$	Elastic right Cauchy Green tensor in the intermediate configuration
$\mathbf{C}^p$	Plastic right Cauchy-Green tensor
D	Phase field variable
$\bar{\mathbf{D}}^p$	Symmetric part of plastic distortion rate
E	Young modulus
$\mathbf{E}$	Green Lagrange strain tensor
$\mathbf{E}^e$	Elastic part of Green Lagrange strain tensor
$\mathbf{E}^p$	Plastic part of Green Lagrange strain tensor
$\mathbf{F}$	Deformation gradient
$\mathbf{F}^e$	Elastic part of the deformation gradient
$\mathbf{F}^p$	Plastic part of the deformation gradient
G_c	Critical energy release rate
$\mathbf{G}$	Metric tensor in the reference configuration
$\mathbf{G}_I$	Basis vector in the reference configuration
$\mathbf{G}^I$	Dual basis vector in the reference configuration
H	Kinematic hardening parameter
I_1	First invariant of Kirchhoff stress tensor
J	Jacobian of deformation gradient

J_2	Second invariant of deviatoric Kirchhoff stress tensor
J_3	Third invariant of deviatoric Kirchhoff stress tensor
K	Bulk modulus
$\bar{\mathbf{L}}^{\mathbf{P}}$	Plastic distortion rate
$\bar{\mathbf{M}}$	Mandel stress
$\mathbf{P}$	First Piola Kirchhoff stress tensor
$\mathbf{R}$	Rotation tensor from polar decomposition of deformation gradient
$\mathbf{S}$	Second Piola Kirchhoff stress tensor
T	Hardening parameter in dynamic recovery term
$\mathbf{V}$	Left stretch tensor
W^e	Elastic energy
W^p	Plastic work
W_{th}	Threshold energy
$\mathbf{X}$	Material point $\mathbf{X} \in \mathbf{B}$
$\mathbf{b}^e$	Elastic left Cauchy Green tensor
$\mathbf{d}$	Deformation tensor
$\mathbf{d}^e$	Elastic deformation tensor
$\mathbf{d}^p$	Plastic deformation tensor
$\mathbf{g}_i$	Basis vector in the spatial configuration
$\mathbf{g}^i$	Dual basis vector in the spatial configuration
$\mathbf{g}$	Metric tensor in the spatial configuration
$\mathbf{l}$	Velocity gradient
l	Length scale parameter
$\mathbf{n}$	Unit normal to yield surface
t	Time
$\mathbf{u}$	Displacement vector
$\mathbf{x}$	Spatial point $\mathbf{x} \in \bar{\mathbf{B}}_t$
$\mathbf{w}$	skew-symmetric part of velocity gradient

CONTENTS

Greek Notations

α	Kinematic hardening tensor
$\mathbf{\Gamma}$	Kinematic hardening tensor in the reference configuration
$\mathbf{\Gamma}^D$	Discontinuity boundary in reference configuration
$\mathbf{\Gamma}_t^D$	Discontinuity boundary in spatial configuration
γ	Plastic Lagrange multiplier
ϵ	Total strain
ϵ_{eq}^p	Equivalent plastic strain
ϵ^p	Plastic strain
ϵ^e	Elastic strain
ϵ^{vp}	Viscoplastic strain
η	Stress triaxiality parameter
θ	Lode angle parameter
μ	Shear modulus
χ	Deformation map
ν	Poisson ratio
ρ_0	Density in the reference configuration
σ	Cauchy stress
τ	Kirchhoff stress
τ_1, τ_2, τ_3	Principal Kirchhoff stresses
τ_y	Yield stress
ϕ	Yield function
ψ	Free energy
Ω	Spin tensor
$\Omega^{\log}$	Logarithmic spin tensor

Calligraphic Letters

$\mathcal{C}$	Algorithmically consistent spatial tangent constitutive tensor
$\mathcal{E}$	Elastic stiffness tensor

Abbreviations/Acronyms

dev	Deviatoric part in the spatial configuration
DEV	Deviatoric part in the reference configuration
tr	Trace part in the spatial configuration
TR	Trace part in the reference configuration

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