

**UNUSUAL COUPLED DEFORMATION AND  
SUPERCOILING IN ELASTIC RODS WITH  
APPLICATION TO BIOMOLECULES**

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INDIAN INSTITUTE OF TECHNOLOGY DELHI  
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APPLICATION TO BIOMOLECULES**

by

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Submitted  
in fulfillment of the requirements of the degree of Doctor of Philosophy  
to the



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*Dedicated To  
My Family and Friends*

# Certificate

This is to certify that the thesis entitled “**Unusual coupled deformation and supercoiling in elastic rods with application to biomolecules**”, being submitted by **Mr. Raushan Singh** to the Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy**, is a record of bonafide research carried out by him under my supervision. The thesis in my opinion, is worthy of consideration in accordance with the rules and regulations of the Institute. To the best of my knowledge, the results embodied in this thesis have not been submitted to any other University or Institute for the award of any other degree or diploma.

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# Abstract

Interest in the theory of rods has been the subject of intense research due to its applicability in several areas of scientific and applied research such as its applicability in biophysics, modeling chiral nanotubes, biomolecules, arteries, cables, ropes, strings etc. Broadly speaking, the present work considers two topics in the context of rods and tubes. The first part of this thesis covers unusual extension-torsion-inflation coupled deformations in helically reinforced tubes. In the second part, we propose efficient numerical techniques for solving the governing equations of rods: (i) a cubic asymptotic numerical method is presented for continuation of static equilibria for elastic rods and (ii) a singular-free numerical technique is presented to model supercoiling of rods having continuously distributed charge over them.

We present a general theory to model coupled extension-torsion-inflation deformation in helically reinforced pressurized circular tubes. Both compressible and incompressible tubes are considered. Furthermore, we present a thin tube formulation in which on applying the thin tube limit, the nonlinear ordinary differential equation to obtain the in-plane radial displacement is converted into a set of two simple algebraic equations for the compressible case and one equation for the incompressible case. This allows us to obtain analytical expressions, in terms of the tube's intrinsic twist, material constants and the applied pressure. Effects of intrinsic twist and material anisotropy on coupled extension-torsion-inflation deformation in circular tubes about their stress-free state and at finite strain are presented. Simple analytical expressions for coupling stiffnesses corresponding to extension-twist, twist-inflation and extension-inflation couplings are also obtained. We show that the sign of the extension-twist coupling stiffness, which governs initial overwinding/unwinding in tubes during their extension, is not just dependent on the tube's intrinsic twist but also on two other parameters: ratio of the Young's moduli in the lateral surface of the orthotropic tube and the excess of the Poisson's ratio from an isotropy condition. By tuning these two parameters, one can generate the counter-intuitive overwinding as reported earlier in the case of DNA. Similarly, we show that even with positive Poisson's ratio, a helically reinforced tube could inflate on being stretched. We further show numerically that such tubes can be tuned to generate initial overwinding followed by rapid unwinding as observed during finite stretching of a torsionally relaxed DNA. Finally, we demonstrate that such tubes can also exhibit usual deflation initially followed by unusual inflation as the tube is finitely stretched.

We then present an efficient numerical scheme based on asymptotic numerical method for the continuation of spatial equilibria of special Cosserat rods. Using quaternions to represent rotation, the equations of static equilibria of special Cosserat rods are posed as a system of thirteen first order ordinary differential equations having cubic nonlinearity. The derivatives in these equations are further discretized to yield a system of

cubic polynomial equations. As asymptotic-numerical methods are typically applied to polynomial systems having quadratic nonlinearity, a modified version of this method is presented in order to apply it directly to our cubic nonlinear system. We then use our method for the continuation of equilibria of a follower load problem and demonstrate our method to be highly efficient when compared to conventional solvers based on the finite element method. Finally, we demonstrate how our method can be used for computing the buckling load as well as for the continuation of post-buckled equilibria of hemitropic rods.

Supercoiling of charged biomolecules is another topic of interest for biological and mechanics community. In this context, we present an efficient formulation which incorporates continuously distributed charge in the equilibrium equations of Kirchhoff rods. The challenge here is to model the electrostatic interaction (Debye-Huckel and Coulomb interaction) which has inverse square singularity in the equivalent continuum approach. In the context of DNA supercoiling, researchers employ discrete approach and model DNA at base-pair level. The discrete approach automatically eliminates singularity. However, as the length of the DNA increases, the ratio of the distance between neighboring base-pairs and the total DNA length approaches zero. Accordingly, the discrete approach starts sensing singularity. We relook at the equivalent continuum problem where the point charges are now continuously distributed. The double summation (in discrete case) over base pair is replaced by double integral (in continuum case) and this double integral is singular. Due to continuously distributed charge, our equilibrium equations of the Kirchhoff rod becomes a system of integro-differential equations and further, due to singularity present in the double integral, the electrostatic energy, the contact force and equilibrium equations all become singular. We make the system of equilibrium equations well posed (singularity free) by carefully doing a Taylor's expansion about the singular point. Finally, we show that our singular-free numerical scheme turns out to be very efficient when compared to the existing discrete approach.

## सार

छड़ के सिद्धांत में रुचि वैज्ञानिक और अनुप्रयुक्त अनुसंधान जैसे जैव-भौतिकी में इसकी प्रयोज्यता, चिराल नैनोट्यूब, बायोमोलेक्यूलस, धमनियों, केबल, रस्सियों, तारों आदि में व्यापक रूप से लागू होने के कारण गहन शोध का विषय है। वर्तमान कार्य छड़ और ट्यूब के संदर्भ में दो विषयों पर विचार करता है। इस थीसिस का पहला हिस्सा असामान्य रूप से प्रबलित ट्यूबों में असामान्य विस्तार-मरोड़- इन्फ्लेशन युग्मित विकृतियों को शामिल करता है। दूसरे भाग में, हम छड़ों के शासी समीकरणों को हल करने के लिए कुशल संख्यात्मक तकनीकों का प्रस्ताव करते हैं: (i) लोचदार छड़ के लिए स्थैतिक संतुलन की निरंतरता के लिए एक घन विषम संख्यात्मक विधि प्रस्तुत की जाती है और (ii) एक सिंगुलरिटी-मुक्त संख्यात्मक तकनीक को छड़ के सुपरकोलिंग को मॉडल करने के लिए प्रस्तुत किया जाता है, जिसमें उनके ऊपर लगातार वितरित प्रभार होते हैं।

हम सामान्य रूप से प्रबलित दबाव वाले परिपत्र ट्यूबों में युग्मित विस्तार-मरोड़-इन्फ्लेशन विरूपण को मॉडल करने के लिए एक सामान्य सिद्धांत प्रस्तुत करते हैं। संपीडित और असंगत दोनों ट्यूबों को माना जाता है। इसके अलावा, हम एक पतली ट्यूब सूत्रीकरण पेश करते हैं जिसमें पतली ट्यूब सीमा को लागू करने पर, इन-प्लेन रेडियल विस्थापन प्राप्त करने के लिए नॉनलाइनियर साधारण अंतर समीकरण को दो सरल बीजगणितीय समीकरणों के लिए संपीडित मामले के एक सेट में परिवर्तित किया जाता है और अपूर्ण के लिए एक समीकरण मामला है। यह हमें ट्यूब के आंतरिक मोड़, सामग्री स्थिरांक और लागू दबाव के संदर्भ में विश्लेषणात्मक अभिव्यक्तियाँ प्राप्त करने की अनुमति देता है। आंतरिक तनाव और उनके तनाव मुक्त राज्य के बारे में परिपत्र ट्यूबों में युग्मित विस्तार-मरोड़-इन्फ्लेशन विरूपण पर आंतरिक मोड़ और सामग्री अनिसोट्रॉपी के प्रभाव प्रस्तुत किए जाते हैं। विस्तार-मोड़, मोड़-इन्फ्लेशन और विस्तार-इन्फ्लेशन युग्मन के अनुरूप युग्मन कठोरता के लिए सरल विश्लेषणात्मक अभिव्यक्तियाँ भी प्राप्त की जाती हैं। हम बताते हैं कि विस्तार-मोड़ युग्मन कठोरता का संकेत, जो उनके विस्तार के दौरान ट्यूबों में प्रारंभिक ओवरवाइंडिंग / अनवाइंडिंग को नियंत्रित करता है, न केवल ट्यूब के आंतरिक मोड़ पर निर्भर करता है, बल्कि दो अन्य मापदंडों पर भी निर्भर करता है: पार्श्व सतह में यंग के मोडुली का अनुपात ऑर्थोट्रोपिक ट्यूब और एक आइसोट्रॉपी स्थिति से पॉइसन के अनुपात की अधिकता। इन दो मापदंडों को ट्यूब करके, डीएनए के मामले में पहले की तरह काउंटर-सहज ज्ञान युक्त ओवरवाइंडिंग उत्पन्न कर सकता है। इसी तरह, हम दिखाते हैं कि पॉजिटिव पॉजिशन के अनुपात के साथ भी, एक मजबूत रूप से प्रबलित ट्यूब को बढ़ाया जा सकता है। हम आगे संख्यात्मक रूप से दिखाते हैं कि इस तरह के ट्यूबों को प्रारंभिक ओवरवाइंडिंग उत्पन्न करने के लिए ट्यूब किया जा सकता है जिसके बाद तेजी से अनवाइंडिंग किया जाता है जैसा कि एक टॉरसली आराम से डीएनए के परिमित खिंचाव के दौरान पाया जाता है। अंत में, हम यह प्रदर्शित करते हैं कि इस तरह की नलिकाएं सामान्य रूप से असामान्य इन्फ्लेशन के बाद भी प्रदर्शित हो सकती हैं क्योंकि ट्यूब बारीक रूप से फैली हुई हैं।

हम तब एक विशेष संख्यात्मक योजना को प्रस्तुत करते हैं जो विशेष कॉंजैरेट छड़ के स्थानिक संतुलन की निरंतरता के लिए असममित संख्यात्मक पद्धति पर आधारित है। रोटेशन का प्रतिनिधित्व करने के लिए कटेनियंस का उपयोग करते हुए, विशेष कॉंजैरेट छड़ के स्थैतिक संतुलन के समीकरणों को तेरह पहले क्रम के सिस्टम के रूप में पेश किया जाता है, जिसमें सामान्य अंतर समीकरण क्यूबिक नॉनलाइनरिटी होते हैं। इन समीकरणों के व्युत्पन्न को आगे चलकर क्यूबिक बहुपद समीकरणों की एक प्रणाली बनाने के लिए विवेकाधीन किया जाता है। जैसा कि स्पर्शान्मुख-संख्यात्मक विधियाँ आमतौर पर बहुपद प्रणालियों में लागू होती हैं, जिसमें द्विघात गैर-विहीनता होती है,

इस विधि का एक संशोधित संस्करण हमारे क्यूबिक गैर-रेखीय प्रणाली में इसे सीधे लागू करने के लिए प्रस्तुत किया जाता है। हम तब एक फॉलोअर लोड समस्या के संतुलन की निरंतरता के लिए अपनी पद्धति का उपयोग करते हैं और परिमित तत्व विधि के आधार पर पारंपरिक सॉल्वरों की तुलना में अत्यधिक कुशल होने के लिए हमारी विधि का प्रदर्शन करते हैं। अंत में, हम यह प्रदर्शित करते हैं कि कैसे हमारे तरीके का उपयोग बकलिंग लोड को कम करने के साथ-साथ हेमट्रोपिक छड़ों के बाद के बकले के संतुलन की निरंतरता के लिए किया जा सकता है।

आरोपित बायोमोलेक्युलस की सुपरकोलिंग जैविक और यांत्रिकी समुदाय के लिए रुचि का एक और विषय है। इस संदर्भ में, हम एक कुशल सूत्रीकरण प्रस्तुत करते हैं जो किर्चॉफ छड़ के संतुलन समीकरणों में निरंतर वितरित प्रभार को शामिल करता है। यहाँ चुनौती इलेक्ट्रोस्टैटिक इंटरैक्शन (डेबी-हकेल और कूलम्ब इंटरैक्शन) को मॉडल करना है जिसने समतुल्य निरंतर दृष्टिकोण में वर्ग विलक्षणता को उलट दिया है। डीएनए सुपरकोलिंग के संदर्भ में, शोधकर्ता बेस-जोड़ी स्तर पर असतत दृष्टिकोण और मॉडल डीएनए को नियुक्त करते हैं। असतत दृष्टिकोण स्वचालित रूप से विलक्षणता को समाप्त करता है। हालाँकि, जैसे-जैसे डीएनए की लंबाई बढ़ती है, पड़ोसी बेस-जोड़ और डीएनए की कुल लंबाई के बीच की दूरी का अनुपात शून्य हो जाता है। तदनुसार, असतत दृष्टिकोण में विलक्षणता की अनुभूति होने लगती है। हम समतुल्य सातत्य समस्या पर ध्यान देते हैं जहाँ बिंदु आवेश अब लगातार वितरित होते हैं। बेस जोड़ी के ऊपर डबल समन (असतत मामले में) को डबल इंटीग्रल (सातत्य मामले में) से बदल दिया जाता है और यह डबल इंटीग्रल विलक्षण होता है। निरंतर वितरित प्रभार के कारण, किर्चॉफ रॉड के हमारे संतुलन समीकरणों में पूर्णांक-अंतर समीकरणों की एक प्रणाली बन जाती है और आगे, दोहरी अभिन्न, इलेक्ट्रोस्टैटिक ऊर्जा, संपर्क बल और संतुलन समीकरणों में मौजूद विलक्षणता के कारण सभी एकवचन बन जाते हैं। हम एकवचन बिंदु के बारे में टेलर के विस्तार को ध्यान से करते हुए संतुलन के समीकरणों को अच्छी तरह से पेश (एकवचन मुक्त) बनाते हैं। अंत में, हम बताते हैं कि मौजूदा असतत दृष्टिकोण की तुलना में हमारी विलक्षण-मुक्त संख्यात्मक योजना बहुत ही कारगर साबित होती है।

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