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Femoral fracture load and fracture pattern is accurately predicted using a gradient-enhanced quasi-brittle finite element model

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ABSTRACT

Nonlinear finite element (FE) modeling can be a powerful tool for studying femoral fracture. However, there remains little consensus in the literature regarding the choice of material model and failure criterion. Quasi-brittle models recently have been used with some success, but spurious mesh sensitivity remains a concern. The purpose of this study was to implement and validate a new model using a custom finite element designed to mitigate mesh sensitivity problems. Six specimen-specific FE models of the proximal femur were generated from quantitative tomographic (qCT) scans of cadaveric specimens. Material properties were assigned *a-priori* based on average qCT intensities at element locations. Specimens were experimentally tested to failure in a stumbling load configuration, and the results were compared to FE model predictions. There was a strong linear relationship between FE predicted and experimentally measured fracture load ($R^2 = 0.79$), and error was less than 14% over all cases. In all six specimens, surface damage was observed at sites predicted by the FE model. Comparison of qCT scans before and after experimental failure showed damage to underlying trabecular bone, also consistent with FE predictions. In summary, the model accurately predicted fracture load and pattern, and may be a powerful tool in future studies.

1. Introduction

Osteoporosis is a significant source of morbidity and mortality, particularly among the elderly [1,2]. To develop effective intervention strategies for the prevention of osteoporotic fractures, it is necessary to identify individuals who are most at risk. This can be challenging, as the likelihood of suffering a fracture is dependent on a number of factors including bone strength, the likelihood of suffering a fall, and the severity of the fall. Finite element (FE) modeling can be a powerful tool to help further understand some of these factors.

Linear FE models are computationally inexpensive, and commonly used [3–6]. Linear models treat bone as a linear elastic solid, and failure is assumed to occur after a certain number of elements exceed the selected failure criterion. These models are able to accurately predict strains at low loads [7], and achieve strong correlations between FE predicted and experimentally determined failure load ($R^2 > 0.77$). Despite the strength of correlation, however, error magnitudes can remain quite large; some studies show that individual specimens have differences of up to 45% between predicted and experimentally measured fracture loads [4,6]. To achieve better results, some FE studies incorporate nonlinear material properties. In these studies, bone elements behave linear-elastically until a failure a condition is met, at which point the element's properties are degraded, *i.e.*, the stiffness and/or stress in the element is adjusted to account for localized failure of the bone material [8–11]. However, there is currently little consensus regarding the best material model and failure criterion to use for modeling failure of the proximal femur.

Some very recent studies [12,13] have had success using a quasi-brittle damage model, where stiffness of elements degrades gradually as strain increases, and the crack is modeled as the region of elements whose stiffness has been reduced to near zero. While the technique is powerful, there are important challenges that need to be addressed. FE models that include strain softening behavior have well documented issues with spurious mesh sensitivity [14,15]. The size of the damaged region corresponds to the size of the mesh used to solve the problem. As the mesh is refined, the size of the damaged region, and thus the energy dissipated, shrinks. This is a physically inadmissible result; the energy dissipated by crack formation is a property of the material and should not be dependent on mesh size [14,15].

To remedy this issue, some authors have proposed using a nonlocal constitutive model. For example, damage evolution can be driven by a weighted spatial averaging of strains near a point,

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rather than the local strain at the point itself. This technique has been used successfully for simulations of vertebral bone [16], but is computationally expensive to implement within a conventional finite element solver. As an alternative, gradient-dependent descriptions have recently gained interest. Using Taylor series expansions, these models approximate the nonlocal parameter as the solution to a differential equation which can be evaluated locally [17]. This equation can be easily coupled to the equation of equilibrium and solved using the finite element method.

While this method has been used successfully in the past to model failures in quasi-brittle engineering materials [18], to the best of the author's knowledge, it has not been used to study bone fracture at the organ level. Thus, the purpose of this study is to develop specimen-specific finite element models of the femur, simulate fracture using a gradient-enhanced quasi-brittle damage model, and validate the predicted fracture load and fracture pattern through experimental testing.

2. Methods

2.1. The nonlocal model

Formulation of the nonlocal model, and its implementation using finite elements, was derived in detail by Peerlings et al. [18], but is summarized here for the reader's convenience. In a quasi-brittle material, stress at a point is a function of both strain and the state of damage:

$$\boldsymbol{\sigma} = (1 - D)\boldsymbol{C}\ \boldsymbol{\varepsilon} \tag{1}$$

where $\boldsymbol{C}$ is the stiffness tensor for the undamaged material, D is the damage parameter, $\boldsymbol{\sigma}$ is the stress tensor and $\boldsymbol{\varepsilon}$ is the strain tensor . The state of damage is related to the loading history; most typically, damage is related to a scalar measure of deformation, known as equivalent strain ε_{eq}, computed from components of the strain tensor. In a nonlocal model, damage is related to a weighted volume average of equivalent strains, computed from:

$$\overline{\varepsilon_{eq}}\left(\vec{x}\right) = \int_V g\left(\vec{\epsilon}\right)\varepsilon_{eq}\left(\vec{x} + \vec{\epsilon}\right)dV \tag{2}$$

where $\overline{\varepsilon_{eq}}(\vec{x})$ is the nonlocal equivalent strain at point $\vec{x}$, $\vec{\epsilon}$ is an integration variable, and $g(\vec{\epsilon})$ is the weighting function. Unfortunately, Eq. (2) is difficult to implement in a traditional finite element solver. However, by manipulating the Taylor series expansion of Eq. (2), Peerlings et al. [18] showed that the nonlocal strain can be approximated using a differential equation:

$$\overline{\varepsilon_{eq}} - c\nabla^2\overline{\varepsilon_{eq}} = \varepsilon_{eq} \tag{3}$$

where c is related to the nonlocal interaction radius [17], and has units of length squared. Eq. (3) is significantly easier to implement and solve using the finite element method.

2.2. The finite element implementation

The custom finite element used in this study simultaneously solves the equation for nonlocal strain (Eq. 3) alongside the familiar equation of static equilibrium with body forces neglected:

$$\nabla \cdot \boldsymbol{\sigma} = 0 \tag{4}$$

Coupling between Eq. (3) and Eq. (4) occurs due to the fact that stress $\boldsymbol{\sigma}$ is related to damage, from the constitutive law (Eq. 1), and damage evolution is computed from nonlocal strains. To solve this system of equations, the unknown fields of displacement ($\mathbf{u}$) and nonlocal strain ($\overline{\varepsilon_{eq}}$) are discretized using two sets of standard finite element shape functions $\boldsymbol{N_u}$ and $\boldsymbol{N_\varepsilon}$:

$$\boldsymbol{u} = \ \boldsymbol{N}_u\ \bar{\boldsymbol{U}} \tag{5}$$

$$\varepsilon_{eq} = \ \boldsymbol{N}_\varepsilon\ \bar{\boldsymbol{\varepsilon}} \tag{6}$$

where $\bar{\boldsymbol{U}}$ and $\bar{\boldsymbol{\varepsilon}}$ are vectors containing the nodal values of displacement and nonlocal equivalent strain, respectively. Analogous to the derivation of a more standard continuum finite element, divergence theorem is used to manipulate Eq. (4) into the weak form. Substitution of Eq. (5) then results in the familiar finite element equations:

$$\boldsymbol{f}_u^{int} = \boldsymbol{f}_u^{ext} \tag{7}$$

$$\boldsymbol{f}_u^{int} = \int (\boldsymbol{B}_u)^T\boldsymbol{\sigma}\ d\Omega \tag{8}$$

$$\boldsymbol{f}_u^{ext} = \int (\boldsymbol{N}_u)^T\boldsymbol{p}\ d\Omega \tag{9}$$

where $\boldsymbol{p}$ is the vector of external nodal forces acting on the body. The matrix $\boldsymbol{B}_u$ is assembled from derivatives of the shape functions $\boldsymbol{N}_u$, and describes the strain–displacement relationship. Similarly, casting the differential equation for nonlocal strain into the weak form, and substituting the discretization Eq. (6), yields:

$$\boldsymbol{K}_{\varepsilon\varepsilon}\ \bar{\boldsymbol{E}} = \ \boldsymbol{f}_e \tag{10}$$

Where:

$$\boldsymbol{K}_{\varepsilon\varepsilon} = \int \boldsymbol{N}_\varepsilon{}^T\boldsymbol{N}_\varepsilon + \ \boldsymbol{B}_\varepsilon{}^T c\boldsymbol{B}_\varepsilon\ d\Omega \tag{11}$$

$$\boldsymbol{f}_e = \int \boldsymbol{N}_\varepsilon{}^T\varepsilon_{eq}\ d\Omega \tag{12}$$

Similar to Eq. (8), the matrix $\boldsymbol{B}_\varepsilon$ is assembled from derivatives of the shape functions $\boldsymbol{N}_\varepsilon$. Damage evolution causes nonlinearity, and so Eqs. (7) and (10) are linearized then solved by Newton–Raphson iterations. For a given set of estimated solution variables $\overline{\boldsymbol{U}_i}$ and $\bar{\boldsymbol{E}}_i$ estimated at iteration i, the updates $\overline{\boldsymbol{U}_{i+1}} = \overline{\boldsymbol{U}_i} + \ \triangle\bar{\boldsymbol{U}}$ and $\bar{\boldsymbol{E}}_{i+1} = \bar{\boldsymbol{E}}_i + \ \triangle\bar{\boldsymbol{E}}$ are computed from:

$$\begin{bmatrix} \boldsymbol{K}_{uu} & \boldsymbol{K}_{u\varepsilon} \\ \boldsymbol{K}_{\varepsilon u} & \boldsymbol{K}_{\varepsilon\varepsilon} \end{bmatrix}\begin{Bmatrix} \overline{\Delta\boldsymbol{U}_i} \\ \Delta\bar{\boldsymbol{\varepsilon}}_i \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{f}_u^{ext} - \boldsymbol{f}_u^{int} \\ \boldsymbol{K}^{\varepsilon\varepsilon}\boldsymbol{\varepsilon}_i \end{Bmatrix} \tag{13}$$

Where:

$$\boldsymbol{K}_{uu} = \int \boldsymbol{B}_u{}^T\ (1 - D)\ \boldsymbol{C}\ \boldsymbol{B}_u\ d\Omega \tag{14}$$

$$\boldsymbol{K}_{u\varepsilon} = -\int \boldsymbol{B}_u{}^T\boldsymbol{C}\ \boldsymbol{\varepsilon}\,\boldsymbol{q}\ d\Omega \tag{15}$$

$$\boldsymbol{K}_{\varepsilon u} = \int \boldsymbol{N}_\varepsilon{}^T\left(\frac{\partial\boldsymbol{\varepsilon}_{eq}}{\partial\boldsymbol{\varepsilon}}\right)^T\boldsymbol{B}_u\ \ d\Omega \tag{16}$$

$$\boldsymbol{K}_{\varepsilon\varepsilon} = \int \boldsymbol{N}_\varepsilon{}^T\boldsymbol{N}_\varepsilon + \ \boldsymbol{B}_\varepsilon{}^T c\boldsymbol{B}_\varepsilon\ d\Omega \tag{17}$$

The term $\boldsymbol{q} = \frac{\partial\boldsymbol{D}}{\partial\boldsymbol{\varepsilon}_{eq}}$ if equivalent strain is increasing, and zero otherwise; this prevents the model from reversing damage if strain decreases. Eq. (13) can be solved with commercially available nonlinear finite element solvers. For this study, the equation was implemented as a custom element in the finite element package ABAQUS, using the user subroutine UEL.

2.3. Specimen specific modeling

Six specimen-specific models were developed from fresh-frozen cadaveric femurs obtained from the University of Ottawa's division of clinical and functional anatomy, after approval from their research ethics board . Three were male (ages 60,64,88) and three were female (ages 82, 88, 68). Three-dimensional FE models of the