Computational Study of Cortical Bone Screw Pullout using the Extended Finite Element Method (XFEM)

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Abstract: *A study of screw pullout from cortical bone has been conducted using the UDMGINI subroutine with the extended finite element method (XFEM). XFEM alleviates mesh dependency when computationally modeling crack initiation and propagation. Cortical bone is a naturally occurring composite with a distinctive aligned microstructure that leads to anisotropic material behavior and damage. In this study, using a UDMGINI subroutine, stress components relative to a predefined osteon orientation were computed and an anisotropic damage criterion was used to determine damage initiation and to predict crack propagation. A 2D model of a single screw embedded in cortical bone was generated. A displacement boundary condition was applied to the top surface of the screw. During pull-out, contact interactions were implemented between the newly formed surfaces during crack propagation, eliminating unphysical over closure of elements. The model predicted the correct patterns of damage and crack propagation for both longitudinal (osteons aligned parallel to screw axis) and transverse (osteons aligned perpendicular to screw axis) pullout tests compared to experimental observations. In both cases crack propagation was predicted in the direction of osteon alignment.*

Keywords: *Screw Pullout, Abaqus/Standard, Extended Finite Element Model (XFEM), Crack Propagation, Damage, Failure.*

1. Introduction

1.1 The Extended Finite Element Method

The extended finite element method (XFEM) is a method developed for computationally modeling crack initiation and propagation while alleviating mesh dependency. It can be implemented to simulate initiation and propagation of a discrete crack along an arbitrary, solution dependent path. Additionally contact interactions can be applied to the newly formed surfaces exposed as a result of crack propagation. Thus the effects of friction between newly exposed surfaces can be accounted for. Previously, work has been conducted and microstructure models developed to model fracture of cortical bone. These models incorporated a damage process that initiated damage within an entire element and when the properties of the element degraded such that they could no longer carry load they were deleted from the mesh nucleating voids within the material that replicated experimentally observed fracture mechanisms (Feerick et al. 2011). The possibility to alleviate mesh dependency within these materials offers an advance on previous models as the density of the meshes becomes less influential. Also a material model that is capable of predicting the correct crack patterns without incorporating a detailed geometry of the microstructure will also facilitate the development of larger macro scale models requiring significantly lower computational power. A limitation of some current cortical bone failure models is that they would be too computationally expensive to incorporate in macro scale models of whole bones. Previous studies that generated models of cortical bone using XFEM incorporated detailed microstructures (Budyn et al. 2010; Abdel-Wahab et al. 2012). If these previously developed models were applied to a macro scale simulation of whole bones the computational demand would not be viable. However in the present study we investigate a new feature of Abaqus 6.11 which now facilitates the use of a user subroutine (UDMGINI) for an anisotropic damage initiation criterion without the need for complex microstructure geometry.

1.2 Cortical Bone

Cortical Bone is a naturally occurring composite, consisting of several constituents that dictate the overall response of the material during loading. In the present study we simplify the complex microstructure of bone to osteons (the fiber) embedded in an interstitial matrix. Osteons consist of a series of concentric cylinders of lamellae with a central vascular canal. Osteons are typically 200 µm and are 1-2mm in length and run parallel to the long axis of the bone. The osteons are surrounded by an interstitial matrix consisting of hydroxyapatite. (Rho et al. 1998; Cowin 2001).

1.3 Screw Pullout

Screws are used for orthopedic applications throughout the human body ranging from fracture fixation plates to spinal fusion rods. Maximizing the screw insertion depth in cortical bone is regarded as a way of significantly increasing the pullout strength of the screw (Pollard et al. 2010). A computational model capable of predicting the failure modes and loads that occur during screw pullout would provide a design tool for the evaluation of future designs as well as design optimization. It is important to understand the failure mechanisms that occur during screw pullout as this may determine the angle of insertion and geometry of screw threads to maximize the holding power of the screw.

2. Materials & Methods

2.1 UDMGINI Failure Criteria

A new feature of Abaqus 6.11 is the ability to incorporate a user subroutine UDMGINI for user defined damage initiation criterion. The user may define as many failure indexes as required. In the present study we define two failure indexes for damage initiation in the x and y directions. Failure index one defines the fiber failure index for initiation. The UTS of the fiber as well as the ultimate shear failure of the fiber is defined by the user. Once the value of $\overline{\sigma_f}$ =1 the damage is initiated.

$$Failure\ Index\ 1:\ \overline{\sigma_f} = \sqrt[2]{\left(\frac{\sigma_{11}}{\sigma_{ff}}\right)^2 + \left(\frac{\sigma_{12}}{\sigma_{f\tau_f}}\right)^2}$$

Where:

$\overline{\sigma_f}$	is the fiber damage initiation criterion
σ_{11}	is the current stress in the local x direction
σ_{12}	is the current stress in the local x-y direction
σ_{ff}	is the UTS of the fiber
$\sigma_{f\tau_f}$	is the shear failure strength of the fiber

Failure index 2 defines the matrix failure index for initiation. The UTS of the matrix as well as the ultimate shear failure of the fiber is defined by the user. Once the value of $\overline{\sigma_m}$ =1 damage is initiated.

$$Failure\ Index\ 2:\ \overline{\sigma_m} = \sqrt[2]{\left(\frac{\sigma_{22}}{\sigma_{mf}}\right)^2 + \left(\frac{\sigma_{12}}{\sigma_{m\tau_f}}\right)^2}$$

Where:

$\overline{\sigma_m}$	is the fiber damage initiation criterion
σ_{22}	is the current stress in the local y direction
σ_{12}	is the current stress in the local x-y direction
σ_{mf}	is the UTS of the matrix
$\sigma_{m\tau_f}$	is the shear failure strength of the matrix

As each of the failure indexes are calculated during an iteration of the simulation an array referred to as FNormal is compiled. This array contains the normal direction to the fracture line for each failure mechanism. This means that as damage is initiated in a particular failure index, the direction in which the crack will initiate is returned by the subroutine. The crack direction is defined in terms of the local orientation assigned to the material. For the present study if failure index 1 (fiber failure) is initiated the crack will propagate in the local y direction, perpendicular to the fiber direction. However, if failure index 2 (matrix failure) is initiated the crack will propagate in the local x direction, parallel to the fiber direction.

2.2 Single Element Tests

2D single element tests were conducted to examine crack propagation based upon osteon alignment. A unit cell geometry was created. The material properties assigned to the model are summarized in Table 1. An orientation was applied to the material so that the local x direction represents the direction of the fibers. A single element was held fixed as shown in Figure 1. The block was held fixed in the x and y directions at the bottom left corner. Also the top left and right hand corners were held fixed in the x direction. A 1mm displacement boundary condition was applied in the vertical direction. Longitudinal (fibers orientated parallel to the direction of loading) and transverse (fibers orientated perpendicular to the direction of loading) simulations were conducted.

All simulations were conducted using Abaqus/Standard 6.11 with a CPS4 element. For simulation of crack growth a process of damage evolution (DE) was applied to the model. Energy dissipation was used to determine crack growth. The value selected for cortical bone energy release was based upon those reported in the literatrure (Abdel-Wahab et al. 2012).

Table 1. Cortical bone material properties.

$\mathbf{E_1}$	17100 MPa	$\boldsymbol{\sigma_{ff}}$	233 MPa
$\mathbf{E_2}$	10100 MPa	$\boldsymbol{\sigma_{f\tau_f}}$	85 MPa
$\mathbf{E_{12}}$	3300 MPa	$\boldsymbol{\sigma_{mf}}$	51 MPa
$\boldsymbol{\nu}$	0.3	$\boldsymbol{\sigma_{m\tau_f}}$	34 MPa
$\mathbf{DE_m}$	0.3 N/mm	$\mathbf{DE_f}$	0.3 N/mm

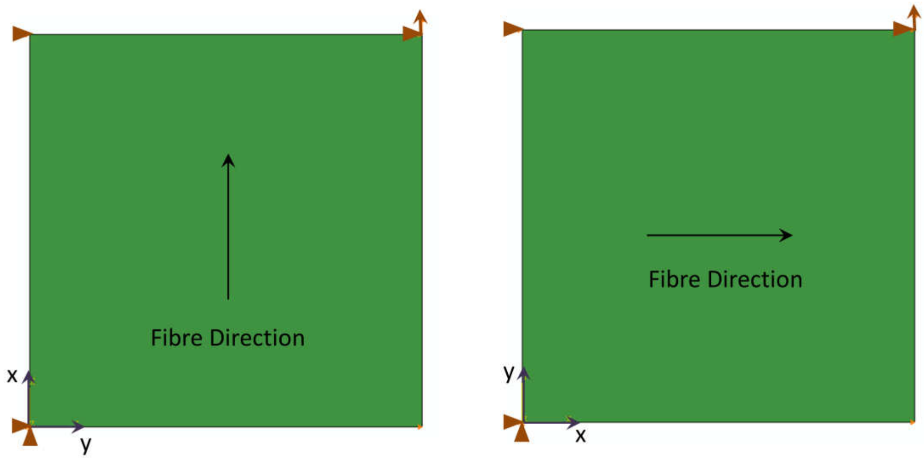

Figure 1. Single element boundary conditions.

2.3 Screw Pullout

A 2D model was developed for screw pullout to illustrate the potential application of XFEM for longitudinal and transverse pullout simulations. A limitation of XFEM is that axisymmetric elements cannot be used with the enrichment feature required for XFEM. Thus a plane stress model is presented here. The boundary conditions applied to the model are shown in Figure 2. A displacement boundary condition of 5mm was applied to the top of the screw. The edge of the screw was held fixed in the global x direction. The edge of the cortical bone was held fixed in both the global x and y directions. Local orientations were applied to assign fiber directions for each simulation. For a longitudinal simulation the fiber direction (local x) was orientated parallel to the axis of the screw. For a transverse simulation the fiber direction (local x) was orientated perpendicular to the axis of the screw. 35,000 CPS4 elements were used with element size of 0.05mm.

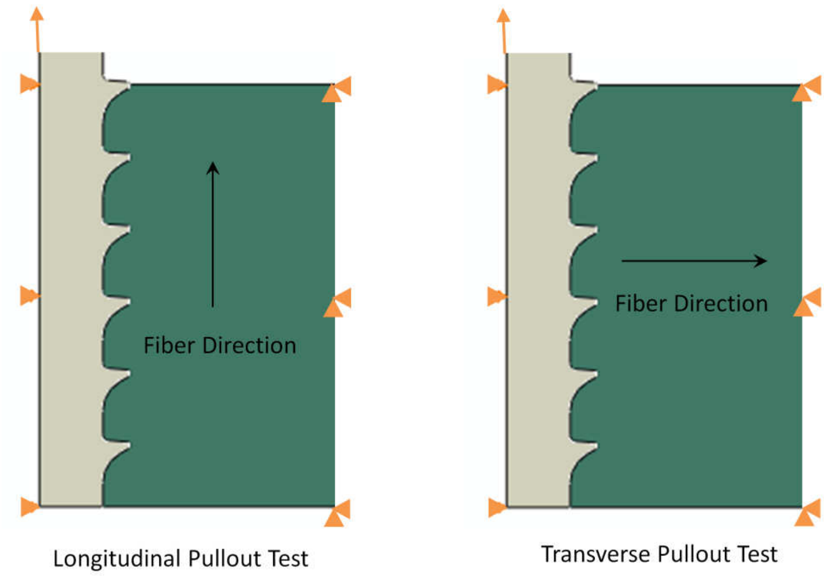

Figure 2. Screw pullout boundary conditions for a longitudinal and transverse simulation.

3. Results

3.1 Single Element Tests

The results for single element simulations are shown in Figure 3. A longitudinal simulation predicts vertical crack formation. A transverse simulation predicts horizontal crack formation. In both a longitudinal and transverse simulation failure index two reaches the value of 1 first. Thus cracks will propagate parallel to the direction of the fiber. Hence, cracks grow in the vertical direction for a longitudinal simulation, while cracks grow in the horizontal direction for a transverse simulation.

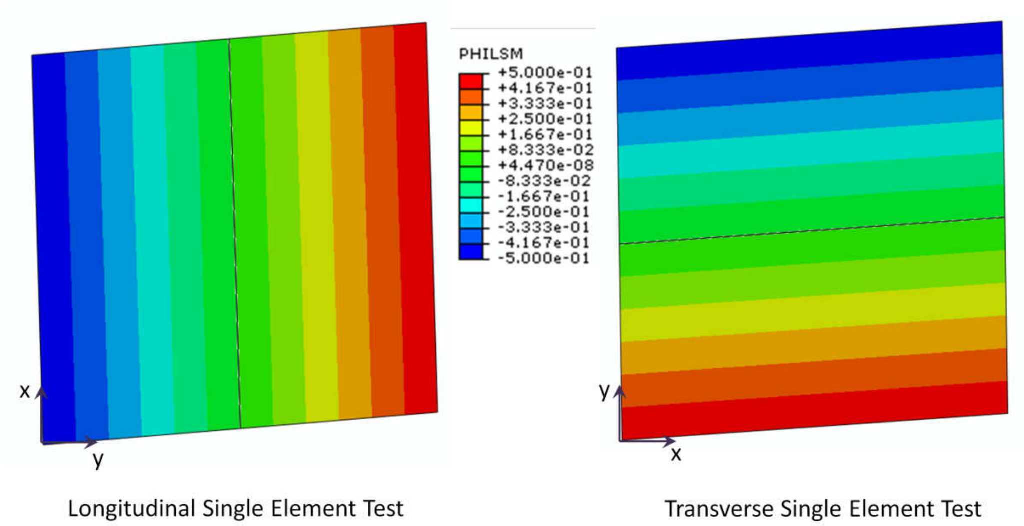

Figure 3. Single element results for longitudinal and transverse simulations.

3.2 2D Screw Pullout Simulation

The results for longitudinal and transverse screw pullout simulations are summarized in Figure 4. A longitudinal pullout simulation predicts localized deformation at the tips of the screw threads. Crack formation is predicted vertically upwards from the screw thread tips with the material between the screw threads removed with the screw leaving no thread definition on the fracture surface. A transverse pullout simulation predicts horizontal crack formation with deformation extending much further into the surrounding bone. In both longitudinal and transverse simulations failure index 2 reaches the value 1 first. For both simulations the cracks propagate parallel to the fiber direction results to significantly different failure modes as the screw is removed from the cortical bone.

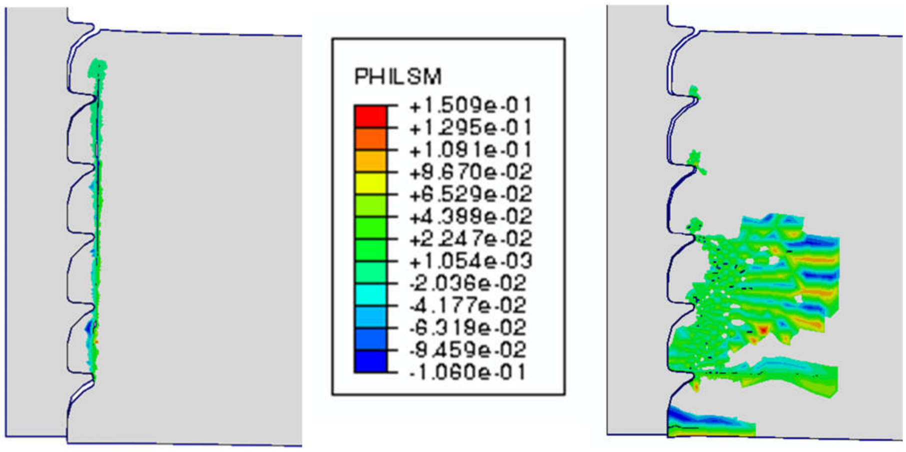

Figure 4. Crack patterns for longitudinal and transverse screw pullout simulations.

4. Discussion

Results highlight the ability of the models to predict significantly different failure mechanisms for cortical bone. This is achieved by simply altering the orientation assigned to the material. It has previously been shown that fracture patterns during screw pullout from cortical bone are dependent upon osteon alignment (Feerick et al. 2011). In the past complex geometries of cortical bone with XFEM have been used to model the alternate fracture patterns of bone depending on osteon alignment (Budyn et al. 2010; Abdel-Wahab et al. 2012). However, in the present study, we have shown that without generating complex microstructure geometry and using the UDMGINI sub routine it is possible to define crack directions based upon the fiber (osteon) orientation.

5. Conclusion

Screw pullout from cortical bone is one example of an application for the UDMGINI subroutine with XFEM. However the same method could be applied to cortical bone simulations for a wide range of orthopedic applications. These applications could range from orthopedic device design evaluation to modeling fracture incidence in whole bones. The use of the model is not limited to applications that consider cortical bone but rather any composite material containing a known fiber alignment.

6. References

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