# Faim Finite Element Analysis Manual

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Version 7.1

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Revision date: September 30, 2015

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## **Chapter 1**

## Introduction

### 1.1 Overview

Faim is a finite element solver optimized for solid mechanics simulations of bone, including strength and stiffness determinations, directly from three-dimensional medical image data such as micro-CT. Faim uses the mesh-free method, which is a highly memory efficient method of finite element analysis. This makes it possible to solve finite element models with very large numbers of degrees of freedom derived directly from high resolution scans.

The Faim Finite Element solver has an established record of being used in scientific studies. See the bibliography for selected studies.

### 1.2 Companion documentation

In addition to this manual, you may want to refer to the following addition documentation, which may be found in the doc directory of your distribution.

- The installation instructions, which depending on your operating system will be one of Faim 7.1 for Windows Installation Instructions.pdf, Faim 7.1 for Linux Installation Instructions.pdf or Faim 7.1 for OS X Installation Instructions.pdf.
- Introduction to the Command Line in OS X.pdf Faim is mostly driven from the command-line. For OS X users unfamiliar with the command line, this short introduction will help with becoming more comfortable with the command line. It also presents a number of time-saving short-cuts. Although specifically targeted to OS X, much of it applies to Linux as well.

### 1.3 How to read this manual

- 1. Start by reading this chapter, Chapter 1. This will give you an brief overview of finite element analysis and the Numerics88 software tools.
- 2. If this is your first time using Numerics88 software, we recommend that you jump first to An introductory tutorial: compressing a solid cube. It will take you through the typical steps of generating a model, verifying it, solving it, and analyzing the results. This is a good introduction to how everything fits together, and will help to put things into context.
- 3. The intervening chapters (before the Tutorials chapter) should be used as reference material. You probably don't want to read them from beginning to end in one sitting with the intention of retaining everything. However, you should at least skim through them, to be aware of the possibilities and options, as well as the limitations and potential pitfalls.
- 4. If you have a lot of data to process, and you already feel comfortable enough working with single models, you will probably want to read the appendix on automating the processing of multiple models with scripts.
- 5. If you are an advanced user who is interested in creating your own custom models, start with the tutorial, Compressing a cube revisited using vtkn88. And then move on to the more advanced tutorials dealing with vtkn88.

### 1.4 Work flow for finite element analysis

There are several steps involved in applying finite element analysis to 3D medical image data. These steps are diagrammed in Figure 1.1. Generally they can be categorized as pre-processing, solving, and post-processing. Faim integrates these steps to simplify the work flow as much as possible, while retaining flexibility and customizability in preparing, solving and analyzing finite element problems derived from micro-CT data.



Figure 1.1: Work flow for FE analysis of micro-CT data.

### 1.4.1 Segmentation

The first step is to segment your 3D medical image data. Although in principle any type of 3D image data can be analyzed, we focus on the use of micro-CT images of bone here. During segmentation, bone and other relevant structures in the CT image are labelled and identified. Segmentation is a very broad and complex field. Because of this, Numerics88 software does not attempt to provide all solutions. Instead, we recommend that you use the segmentation tool provided by the manufacturer of your medical image equipment. This has the advantage that it will be well-integrated into the scanning workflow. In the case of Scanco systems, the tool is *Image Processing Language (IPL)*; for Skyscan systems, *CT-analyzer* provides segmentation functionality.

In cases where your segmentation problem is unusually tricky and beyond the abilities of the manufacturer's tools, there are many third party solutions available.

Whichever tool you use to perform the segmentation, the result should be a 3D image file with integer values. These integer values are referred to as "Material IDs", because they will subsequently be associated with abstract mathematical material models. Material ID zero indicates background material (often air, but sometimes also other material, such as marrow in bone) that can be assumed to have negligible stiffness. Voxels with material ID zero will not be converted to elements in the FE model. Other values can be associated freely with particular materials or material properties as required.

### 1.4.2 Model generation

Model generation is the process of converting a segmented image to a geometrical representation suitable for finite element analysis, complete with suitable constraints such as displacement boundary conditions and applied loads.

A number of steps are required for complete model generation.

### Meshing

Meshing is the process of creating a geometric representation of the model as a collection of finite elements. For micro-CT data, we typically convert each voxel in the input image to a hexahedral (box-shaped) element in the FE model. Each of the corners of the voxel becomes a node in the FE model. Voxels labelled as background (*e.g.* 0) are ignored.

#### Tip

There may be scenarios in which it is desirable to have FE models that have elements smaller or larger than the voxels of the available image. Larger elements lead to smaller FE models (*i.e.* fewer degrees of freedom) which may solve faster, at the expense of accuracy. Smaller elements allow the forces and displacements to vary more smoothly (that is, with higher resolution) in the FE model, at the cost of increased solution time and memory requirements. To alter the FE model from the original 3D image, one typically resamples the original image to the desired resolution employing some sort of interpolation.

#### **Material Assignment**

Material assignment is the process of mapping material IDs to mathematical models for material properties. For example, an isotropic material is specified by its Young's modulus (E) and Poisson's ratio (v).

### **Assigning Boundary Conditions and Applied Loads**

Boundary conditions and applied loads implement a specific mechanical test. The tool used will typically translate a desired physical action, such as a force or a displacement applied to a specific surface, into a set of constraints on a set of nodes or elements.

Faim provides two tools for model generation:

### n88modelgenerator

n88modelgenerator is a program that can generate a number of standard tests (e.g. axial compression, confined compression, etc...). n88modelgenerator has a number of options that allow for flexibility in tweaking these standard models. n88modelgenerator is the easiest method of generating models.

### vtkn88

vtkn88 is a collection of custom VTK objects that you can use for creating models, and is a more advanced alternative to using n88modelgenerator. In order to use them, you need to write a program or script (typically in Python). Some learning curve is therefore involved, as well as the time to write, debug and test your programs. The advantage is nearly infinite customizability. VTK objects, including vtkn88 objects, are designed to be easily chained together into execution pipelines. In this documention, we will give many examples of using vtkn88 in Python scripts.

### 1.4.3 Finite element solver

The finite element solver takes the input model and calculates a solution of the displacements and forces on all the nodes, subject to the specified constraints.

As finite element models derived from micro-CT can be very large, the memory efficiency and speed of the solver are important. Faim uses a mesh-free preconditioned conjugate gradient iterative solver. This type of solver is highly memory efficient.

### Note

Faim is currently limited to small-strain solutions of models with linear and elastoplastic material definitions. This is adequate for most bone biomechanics modelling purposes, as bone undergoes very little strain before failure. However, if you need to accurately model large deformations, the Faim solver is not an appropriate tool.

### 1.4.4 Post-processing and visualization

Post-processing and visualization can take many different forms, depending on the goals of your analysis. For example, you may want to identify locations of stress variations, in which case, a visualization tool is likely the best approach. Or, you may want to obtain a basic output such as an overall stiffness. A number of common post-processing operations are performed by Faim.

Visualization is important even in cases where ultimately you want one or more quantitative values. Visualization provides a conceptual overview of the solution, and may allow one to quickly identify incorrect or invalid results due to some deficiency in the input model. Many visualization software packages exist. If you don't have an existing favourite package, we recommend the use of ParaView, which is an open-source solution from Kitware. The Faim distribution includes plug-ins for ParaView which allow ParaView to directly open Faim file types.

### 1.5 A note about units

Faim is intrinsically unitless; you may use any system of units that are self-consistent.

Nearly all micro-CT systems use length units of millimetres (mm). With forces in Newtons (N), the consistent units for pressure are then megapascals (MPa), as  $1N/(1mm)^2 = 1MPa$ . Young's modulus is an example of a quantity that has units of pressure. In the examples, we will consistently use these units (mm, N, MPa).

### 1.6 Setting environment variables

To use the Faim software, you must first set some environment variables on your workstation. The method of doing this depends on your operating system.

### 1.6.1 On Microsoft Windows

A script to modify the environment variables must be called before running any other components of Faim. This script is set env.bat. Running the script requires knowing the installation directory of Faim. On Windows, the most common installation location is the C:\Program Files directory, in which case we the setenv.bat script can be run as

"C:\Program Files\Faim 7.1\setenv"

Important
setenv.bat does

setenv.bat does not permanently modify the paths on your system; it only changes the environment variables of the current Command Prompt window. You will need to re-run the setenv.bat script in every new Command Prompt window in which you want to use the Faim software.

For convenience, we provide a shortcut to a Faim 7.1 Command Prompt, which can be found in the installation directory. This command prompt automatically calls the setenv.bat script. We suggest that you copy this shortcut to, for example, your desktop. You can then customize it by right-clicking, and choosing Properties from the Pop-up menu. You can for example change the "Start in" location to the directory that you typically use to do FE calculations. In any case, if you have installed Faim to somewhere other than the standard location *sC:\Program Files\Faim 7.1*, then you will have to modify the "Target" line to reflect the actual location of Faim. You can add this shortcut to the start menu by right-clicking and choosing "Pin to Start".



### 1.6.2 On OS X and Linux

A script to modify the environment variables must be called before running any other components of Faim. This script is setenv.sh. Running the script requires knowing the installation directory of Faim. On OS X, the most common installation location is the Applications folder, in which case the setenv.sh script can be called as

source "/Applications/Faim 7.1/setenv.sh"

On Linux, a common installation location is the /opt directory, in which case the command is

source /opt/faim-7.1/setenv.sh

The setenv.sh script will attempt to remove references to other versions of Faim software from the paths, as well as other installations of VTK. However, as every system is unique, it does not in every case correctly identify conflicts in the paths. In rare cases, you may have to adjust the paths by hand.



#### Important

setenv.sh does not permanently modify the paths on your system; it only changes the environment variables of the current shell (Terminal). You will need to re-run the setenv.sh script for every new Terminal instance in which you want to use Faim software.

## **Chapter 2**

## **Preparing Finite Element Models With n88modelger**

### 2.1 Running n88modelgenerator

n88modelgenerator is a tool to create a number of different standard mechanical test simulations directly from segmented 3D images. This tool is designed to be simple to use and in many cases, requires no more than specifying a test type and an input file, like this

n88modelgenerator --test=axial mydata.aim

This will generate a file mydata.n88model that is suitable as input to the Faim solver.

#### Tip

For an introduction to n88modelgenerator, we recommend that you start first with An introductory tutorial: compressing a solid cube. Getting your hands dirty as it were with the program is often the best way to learn. Once you have some familiarity with the program, the following documentation will be make much more sense.

The models produced by n88modelgenerator can be modified and tuned by specifying a number of optional parameters. For example, here n88modelgenerator is run to create an axial test with a specified compressive strain and Young's modulus:

n88modelgenerator --test=axial --normal\_strain=-0.01 --youngs\_modulus=6829 test25a.aim

Parameters can be specified either on the command line, or in a configuration file. Command line arguments must be preceded with a double dash (--). The argument value can be separated from the argument name with either an equals sign (=) or a space. A complete list of all possible arguments is given in the Command Reference chapter. You can also run n88modelgenerator with the --help option to get a complete list of possible parameters. All parameters except the input file name are optional; a default value will be used for unspecified parameters. To use a configuration file, run n88modelgenerator as follows.

n88modelgenerator --config=mytest.conf test25a.aim

Here we are specifying the name of the input file on the command line. This is convenient if we want to use the same configuration file for multiple input files. It is also possible to specify the name of the input file in the configuration file, using the option input\_file. The output file name is left unspecified, so a default value will be used (test25a\_axial.n88model in this case), but it can also be specified either on the command line or in the configuration file if desired.

The configuration file format is one line per option: the parameter name (without leading dashes), followed by the equals character (=), followed by the parameter value. Lines beginning with # are ignored. The following configuration file is exactly equivalent to the example above using command line parameters.

### Example configuration file for n88modelgenerator

```
# This is the example configuration file "mytest.conf"
test = axial
normal_strain = -0.01
youngs_modulus = 6829
```

#### Note

If a parameter is specified on both the command line and in a configuration file, the command line value takes precedence.

n88modelgenerator can accept several different input file formats. Refer to the Command Reference chapter for details.

#### Tip

If you have an input image in a different format, there are many possible solutions. One is to convert the file format, possibly with ParaView, which can read a large number of formats. VTK can also be used to convert many image files. For example, the following python script will convert a MetaImage format file to a VTK .vti file.

```
import vtk
reader = vtk.vtkMetaImageReader()
reader.SetFileName ("test.mhd")
writer = vtk.vtkXMLImageDataWriter()
writer.SetFileName ("test.vti")
writer.SetInputConnection (reader.GetOutputPort())
writer.Update()
```

For more information on scripting, refer to Preparing Finite Element Models With vtkn88.

### 2.2 Test orientation

To allow for flexibility in defining the orientation of applied tests, two coordinate frames are defined:

#### **Data Frame**

The Data Frame is the coordinate frame of the data. The input and output data use the same coordinate system.

#### Test Frame

The Test Frame is the coordinate frame in which the test boundary conditions are applied. Tests are defined with a constant orientation in the Test Frame.

The relationship between the Test Frame and the Data Frame is set by the value of the parameter test\_axis according to the following figure. In the figure, the red-colored axis is the test axis. What this implies exactly depends on the kind of test that is being applied. For example, for a compression test, the direction of compression is along the test axis. The test axis is always the z axis in the Test Frame, and always equal to value of the parameter test\_axis in the Data Frame. The default value for test\_axis is z; for this case the Test Frame and the Data Frame coincide, as shown.



Figure 2.1: Coordinate frames Test Frame and Data Frame as set by the option test\_axis.

In the test descriptions, references to "Top" refer to the maximum z surface in the Test Frame; References to "Bottom" refer to the minimum z surface in the Test Frame. Likewise "Sides" refers to the surfaces normal to the x and y axes in the Test Frame.

The Test Frame is used only for the specification of tests (*i.e.* a specific configuration of boundary conditions and applied loads) within n88modelgenerator and vtkn88. When the model is written to disk as an n88model file, it is encoded with reference to the original Data Frame. As a consequence post-processing and visualization are in the original Data Frame.

#### Note

In terms of rotations, for a setting of test axis = x, the transformation from the Test Frame to the Data Frame is a rotation of  $-90^{\circ}$  about the x axis, followed by a  $-90^{\circ}$  rotation about the z' axis. For a setting of test axis = y, the transformation from the Test Frame to the Data Frame is a rotation of  $90^{\circ}$  about the y axis, followed by a  $90^{\circ}$  rotation about the z' axis. These transformation from the Test Frame to the Data Frame is a rotation of  $90^{\circ}$  about the y axis, followed by a  $90^{\circ}$  rotation about the z' axis. These transformation sequences are of course not unique. For most applications, it is not necessary to know these transformations; it should be sufficient to refer to Figure 2.1.

### 2.3 Standard tests

## Important

Axis directions in the following test descriptions are in the Test Frame. All the standard tests can be applied along any axis of the data by specifying test\_axis, as described in the previous section.

### 2.3.1 Uniaxial test

A uniaxial test is a compression (or tension) test with a fixed displacement or force applied along the z axis. Two boundary conditions are applied:

- 1. Nodes on the bottom surface are fixed in the z direction, but free in the x and y directions.
- 2. Nodes on the top surface are subject to a fixed displacement in the z direction. No constraints are applied to the x and y directions.

A uniaxial test is shown in Figure 2.2, along with other types of compression tests. The coordinate system shown in the figure is the Test Frame. A uniaxial test is distinguished from an axial test (described below) by the fact that nodes on the top and bottom surfaces are unconstrained laterally. This corresponds to zero contact friction.

The amount of displacement applied to the top surface can be specified by either the normal\_strain or displacement parameters.

#### Important

Uniaxial models are under-constrained since, as defined, arbitrary lateral motion, and arbitrary rotation about the *z* axis of the entire model are permitted. This results in a singular system of equations. A "pin" may be added to prevent these motions. See pin parameter. However, Faim will find a (non-unique) solution even without a pin, and in fact typically does so faster in the absence of a pin. A pin should always be added if you want to use an algebraic solver, or if you intend to compare the absolute positions of multiple solved models. Alternatively, you can register the solved models before comparing absolute positions.



Figure 2.2: Compression tests.

### 2.3.2 Axial test

An axial test is similar to a uniaxial test, with the additional constraint that nodes on the top and bottom surfaces are also laterally fixed (*i.e.* no movement of these nodes is permitted in the x-y directions). This corresponds to 100% contact friction.

An axial test is shown in Figure 2.2.

### 2.3.3 Confined test

A confined test is similar to an axial test, with the addition that nodes on the side surfaces of the image volume are constrained laterally (i.e. no movement of these nodes is permitted in the x-y directions).

A confined test is shown in Figure 2.2.

### 2.3.4 Symmetric shear test (symshear)

In a symmetric shear test, the side surfaces are angularly displaced to correspond to a given shear strain. This is shown in Figure 2.3. The only parameter of relevance to a symmetric shear test is shear\_strain.



Figure 2.3: symshear test. The side faces (shaded) are displaced as shown.

### 2.3.5 Directional shear test (dshear)

In a directional shear test, the top surface is displaced laterally, as shown in Figure 2.4. The direction and degree of displacement are set by the parameter shear\_vector, which gives the x, y shear displacement in the Test Frame. Typically shear\_vector is unitless, and the actual displacement is the shear vector scaled by the vertical height of the model (*i.e.* the image extent in the z direction in the Test Frame). If however scale\_shear\_to\_height is set to off, then shear\_vector is taken to have absolute units of length.



Figure 2.4: dshear test. The upper shaded area represents the rigidly translated boundary surface defined by the shear vector (blue).

### 2.3.6 Bending test

In a bending test, the top and bottom surfaces are rotated in opposite directions, as shown in Figure 2.5. The rotation axes are defined by a neutral axis, given by a point in the x,y plane (shown as C) and an angle in the x,y plane. (The coordinate system shown in the figure is the Test Frame.) The neutral axis, projected onto the top and bottom surfaces, is indicated in blue in Figure 2.5. The point and angle defining the neutral axis can be set in n88modelgenerator with the parameters central\_axis and neutral\_axis\_angle respectively. The central axis (point C) can be specified as a numerical x,y pair, or as the center of mass or the center of the data bounds; center of mass is the default setting. The default angle of the neutral axis is 90°, parallel to the y-axis. The amount of rotation can be specified with the parameter bending\_angle. The top and the bottom surfaces are each rotated by half of this value. Positive rotation is defined as in Figure 2.5.

In a bending test, the top and bottom surfaces are laterally constrained; no x,y motion of the nodes on these surfaces is permitted.



Figure 2.5: bending test. The shaded areas represent the rigidly rotated boundary surfaces about the neutral axes (in blue). The neutral axes are defined by the central axis (C-C') and an angle in the x-y plane.

### 2.3.7 Torsion test

In a torsion test, the top surface is rotated about the center axis, as shown in Figure 2.6. The angle of rotation is given by twist\_angle. In the figure positive rotation is shown. The central axis lies parallel to the z axis in the test frame; its position can be specified with the parameter central\_axis. The default position of the central axis is passing through the center of mass.





### 2.4 Uneven surfaces

The grey planes in Figure 2.2 represent the top and bottom boundary surfaces of the image volume. The actual surface to which boundary conditions are applied is by default that part of your object which passes through these boundaries. If your object does not intersect with the top and bottom boundaries of the image volume, then no boundary conditions can be applied using this method.

An alternative is to make use of the parameters top\_surface and bottom\_surface. The "uneven surface" near a boundary is defined as the surface visible from that boundary (viewed from an infinite distance). Visibility is evaluated using ray tracing. Thus for a porous material such as bone the "uneven surface" consists of nodes on the top visible surface, not including nodes on surfaces down inside the pores.

The visible setting can be used for any type of test except symshear. For example, if used with a bending test, the the boundary conditions are no longer exactly tilted planes as shown in figure Figure 2.5; the displacement of each node on the visible surfaces is still calculated as described from its x,y coordinates, but the displaced nodes no longer lie all on a plane (because the initial positions are not on a plane.)

Because the visibility test may find some surfaces far from the boundary in question, it should usually be used together with the parameters bottom\_surface\_maximum\_depth and/or top\_surface\_maximum\_depth. These provide a limit, as a distance from the boundary, for the search for the uneven surface.

### 2.5 Material specification

Material specification consists of two parts:

### **Material Definition creation**

One or more material definitions are created. A material definition is a mathematical description of material mechanical properties. It has a definite type (e.g. linear isotropic or linear orthotropic) and specific numerical values relevant to that type (e.g. a linear isotropic material definition will have particular values of Young's modulus and Poisson's ratio).

### **Material Table generation**

The material table maps material IDs, as assigned during segmentation, to material definitions. It is possible to combine different types of materials (e.g. isotropic and orthotropic) in the same material table. A single material definition can be assigned to multiple material IDs.

In Numerics88, material definitions are indexed by name. This is not evident in n88modelgenerator, as the names are generated automatically, and are not needed by the user. However later we will see how vtkn88 can manipulate material definitions, which it accesses by name.

### 2.5.1 Elastic material properties

Linear elastic materials obey Hooke's Law,

$$\begin{bmatrix} \boldsymbol{\varepsilon}_{xx} \\ \boldsymbol{\varepsilon}_{yy} \\ \boldsymbol{\varepsilon}_{zz} \\ \boldsymbol{\gamma}_{yz} \\ \boldsymbol{\gamma}_{zx} \\ \boldsymbol{\gamma}_{xy} \end{bmatrix} = \mathbf{S} \begin{bmatrix} \boldsymbol{\sigma}_{xx} \\ \boldsymbol{\sigma}_{yy} \\ \boldsymbol{\sigma}_{zz} \\ \boldsymbol{\sigma}_{yz} \\ \boldsymbol{\sigma}_{zx} \\ \boldsymbol{\sigma}_{xy} \end{bmatrix}$$

where  $\varepsilon_{xx}$ ,  $\varepsilon_{yy}$ ,  $\varepsilon_{zz}$  are the *engineering normal strains* along the axis directions,  $\gamma_{yz}$ ,  $\gamma_{zx}$ ,  $\gamma_{xy}$  are the *engineering shear strains*, and  $\sigma_{ij}$  are the corresponding stresses. **S** is the compliance matrix. The inverse of **S** gives  $\sigma$  in terms of  $\varepsilon$ , and is the stiffness matrix **C**.

### **Isotropic materials**

An isotropic material has the same mechanical properties in every direction. Elastic isotropic materials are characterized by only two independent parameters: Young's modulus (E) and Poisson's ratio (v). The compliance matrix is

$$\mathbf{S} = \frac{1}{E} \begin{bmatrix} 1 & -\mathbf{v} & -\mathbf{v} & 0 & 0 & 0 \\ -\mathbf{v} & 1 & -\mathbf{v} & 0 & 0 & 0 \\ -\mathbf{v} & -\mathbf{v} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1-\mathbf{v}) & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(1-\mathbf{v}) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1-\mathbf{v}) \end{bmatrix}$$

For n88modelgenerator the isotropic elastic parameters are set with youngs\_modulus and poissons\_ratio. The default values are 6829 MPa and 0.3, as reported by MacNeil and Boyd (2008).

An isotropic material definition is the default, and will be assumed if no other material type is specified.

### **Orthotropic materials**

Orthotropic elastic materials have two or three mutually orthogonal twofold axes of symmetry. The compliance matrix is

	$\int 1/E_x$	$-v_{yx}/E_y$	$-v_{zx}/E_z$	0	0	0 ]
	$-v_{xy}/E_x$	$1/E_y$	$-v_{zy}/E_z$	0	0	0
c	$-v_{xz}/E_x$	$-v_{yz}/E_y$	$1/E_z$	0	0	0
3 =	0	0	0	$1/G_{yz}$	0	0
	0	0	0	0	$1/G_{zx}$	0
	0	0	0	0	0	$1/G_{rv}$

where

$$E_i$$
is the Young's modulus along axis  $i$ , $v_{ij}$ is the Poisson's ratio that corresponds to a contraction in direction  $j$  when an extension is applied in  
direction  $i$ , $G_{ij}$ is the shear modulus in direction  $j$  on the plane whose normal is in direction  $i$ . It is also called the

Note that the  $v_{ij}$  are not all independent. The compliance matrix must be symmetric, hence

modulus of rigidity.

$$-\mathbf{v}_{yx}/E_y = -\mathbf{v}_{xy}/E_x ,$$
  

$$-\mathbf{v}_{zy}/E_z = -\mathbf{v}_{yz}/E_y ,$$
  

$$-\mathbf{v}_{xz}/E_x = -\mathbf{v}_{zx}/E_z .$$

Therefore only 9 independent parameters are required to fully specify an orthotropic material.

For n88modelgenerator the orthotropic elastic parameters are set with orthotropic\_parameters. Whenever this parameter is specified, an orthotropic material definition will be used.

Note

An orthotropic material defined with a compliance matrix as given above necessarily has its axes of symmetry aligned with the coordinate axes. In contrast, an orthotropic material which is rotated relative to the coordinate axes has a more general form of compliance matrix. In Numerics88 software, such a non-aligned orthotropic material must be specified as an anisotropic material. A rotation matrix relates elements of the anisotropic compliance matrix to the orthotropic compliance matrix. If you want the mathematical details, please contact us!

### Anisotropic material

The most general form of an elastic material is anisotropic, for which we allow the stiffness matrix, or the compliance matrix, to have arbitrary values. The stiffness matrix is symmetric, therefore an anisotropic material requires 21 parameters to define.

Due to the inconvenience of specifying so many parameters in a command-line tool, anisotropic materials cannot be defined in n88modelgenerator. However, if anisotropic materials are required, vtkn88 can be used.

### 2.5.2 Plasticity

Elastoplastic material behaviour is an idealisation of a particular kind of nonlinear stress-strain relationship in which we divide the stress-strain relationship into two clearly distinguished regions: (1) an elastic region, which is identical to the linear elastic material behaviour described above, and, (2) a purely plastic region. For a material subject to a uniaxial deformation, this is sketched in Figure 2.7. In Figure 2.7A, we see the initial elastic region, which in this sketch is tensile, with slope equal to the Young's modulus. This region continues until the stress reaches the yield strength, *Y*. For further increases in strain beyond this point, the stress ceases to increase, and remains constant at the yield strength. The incremental strain in this region is referred to as the plastic strain. Although we must perform work to produce a plastic strain, the plastic strain is irreversible, as can be seen in Figure 2.7B. In B, after applying a large plastic strain, the strain is gradually reduced. The plastic strain component is unchanged during the relaxation; instead, it is the elastic component of the strain that is reduced. As the stress depends entirely on the elastic component of the strain, the stress also immediately begins to decrease. Hence, we do not travel back along the "outward" path, but instead return along a shifted version of the linear elastic region: the material exhibits *hysteresis*. Although the initial point and the final point of Figure 2.7B are both characterised by zero strain, the stress becomes negative - a compressive stress - until, once again, we reach the yield strength limit. Note that the yield strength in tension and the yield strength in compression are not necessarily equal.



Figure 2.7: Elastoplastic behaviour in one dimension.

In three dimensions, an elastoplastic material is characterised by a yield surface, which is the boundary of the elastic region. The yield surface is defined in stress space (or equivalently in strain space). For isotropic materials, the yield surface is most easily defined in the space of the three principal stresses. Stresses lying inside the yield surface are associated with an elastic state. When the stress reaches the yield surface, the material yields, and further increases in strain result in the stress state moving along the yield surface. Many different shapes of yield surface are possible, and are characteristic of different kinds of materials. Yield surfaces are conveniently defined mathematically by a yield function f, such that the yield surface is the locus of points for which f = 0. A complete explanation of elastoplastic behaviour in three dimensions is not given here. We recommend that you consult a good mechanics of materials textbook.

To specify an elastoplastic material, it is necessary both to specify its elastic properties, and its plasticity. Currently, in version 7 of Faim, plasticity can only be used with isotropic elastic properties. Therefore, a typical specification of an elastoplastic model using n88modelgenerator will look something like this

```
n88modelgenerator --youngs_modulus=6829 --poissons_ratio=0.3 --plasticity=vonmises,50 \leftrightarrow mydata.aim
```

The currently supported plastic yield criteria are described below.

### von Mises yield criterion

The von Mises yield criterion states that yielding begins when the distortional strain-energy density attains a certain limit. It is therefore also called the *distortional energy density* criterion. The distortional strain-energy density is the difference between the total strain energy density and the strain energy density arising only from the part of the strain resulting in a volume change. Hence, the distortional strain-energy density is associated with that part of the strain that results in no volume change: or, in other words, the part of the strain that causes a change in shape.

The yield function for a von Mises material, in terms of the three components of the principal stress, is given by

$$f = \frac{1}{6} \left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right] - \frac{1}{3} Y^2$$

The parameter *Y* is the yield strength in uniaxial tension (or compression).

To specify a von Mises material in n88modelgenerator, use the parameter plasticity. For example, --plasticity=vonmises, 68 will define a von Mises material with Y = 68. The units of Y are the same as stress, so typically MPa.

### **Mohr-Coulomb yield criterion**

The Mohr-Coulomb yield criterion is a refinement of the Tresca yield condition, which states that yielding begins when the shear stress at a point exceeds some limit. To this, the Mohr-Coulomb criterion adds a dependence on the hydrostatic stress, such that the shear stress limit is dependent on the hydrostatic stress, in particular that the shear stress limit increases with hydrostatic stress. The Mohr-Coulomb yield criterion is characterised by two values: the cohesion *c* and the angle of internal friction  $\varphi$ . For principal stresses in the order  $\sigma_1 > \sigma_2 > \sigma_3$ , the Mohr-Coulomb yield function is

$$f = \sigma_1 - \sigma_3 + (\sigma_1 + \sigma_3)\sin\phi - 2c\cos\phi$$

Under uniaxial tension, the yield strength is

$$Y_T = \frac{2c\cos}{1+\sin\phi}$$

while under uniaxial compression, the yield strength is

$$Y_C = \frac{2c\cos}{1-\sin\phi}$$

Mohr-Coulomb materials are specified to n88modelgenerator using these two yield strengths. See plasticity. For example, --plasticity=mohrcoulomb, 40, 80 will define a Mohr-Coulomb material with  $Y_T = 40$  and  $Y_C = 80$ . The units of  $Y_T$  and  $Y_C$  are the same as stress, so typically MPa.

### 2.5.3 Material table generation

n88modelgenerator allows the input of only one material definition (vtkn88 by contrast is unlimited). However, one of two types of material table may be chosen: a simple table, consisting of a single material definition, and a more complicated table, for which the input material is scaled in increments, resulting in a whole sequence of material definitions, each of which is a scaled version of the input material.

The type of material table is specified in n88modelgenerator with the parameter material\_table.

### Homogeneous material table

The simplest material table consists of a single material definition. Thus it corresponds to homogeneous material properties: all elements are assigned the same material properties.

Note that although only a single material definition is created, it is nevertheless still possible for the material table to have multiple entries corresponding to multiple material IDs. In this case every material ID in the table maps of course to the same single material definition. n88modelgenerator automates this: it examines the segmented input image, and generates one entry in the material table for every unique material ID (*i.e.* image value) present in the segmented image. Clearly, as a matter of efficiency and simplicity, if you intend to use a image for analysis with homogenous material properties, it is preferable to segment the image object to a single material ID. It is not however, necessary to do so.

#### Homminga material table

Homminga (2011) introduced a model that attempts to account for varying bone strength with density. In this model, the modulii vary according to the equation

$$E = E_{max} (\rho / \rho_{max})^{1.7}$$

Where  $\rho$  is the CT image density. For the orthotropic case, the shear modulii follow the same scaling, and for the anisotropic case, the stiffness matrix follows this scaling.

To use this type of material table, the data must be segmented such that the material ID of each voxel is proportional to its CT image density. As material IDs are discrete, the CT image density is therefore binned. Hence

$$E = E_{max} (ID/ID_{max})^{1.7}$$

 $ID_{max}$  is set with the parameter homminga\_maximum\_material\_id, and the exponent is set with the parameter homminga\_modulus\_exponent.

 $E_{max}$  will depend on the specified material. For an isotropic material, it will be given by youngs\_modulus. However orthotropic or anisotropic materials may also be scaled: the entire stiffness matrix scales according to the above-stated law.

### Warning

In contrast to the homogenous material table, a Homminga material table is not guaranteed *a priori* to have an entry for every material ID present in the input segmented image. If your segmented image has material IDs larger than the specified  $ID_{max}$ , n88modelgenerator will produce an error.

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## **Chapter 3**

## **Preparing Finite Element Models with vtkn88**

You only need to read this chapter if you are interested in writing scripts to create your own custom model types. For many users, n88modelgenerator, as described in the previous chapter, will be sufficient.

Although n88modelgenerator can generate many useful models for FE analysis, at times additional flexibility is required. In order to provide as much flexibility to the user as possible, we provide the option for users to perform custom model generation. This functionality is provided by vtkn88 toolkit, which is built on VTK . VTK is "an open-source, freely available software system for 3D computer graphics, image processing and visualization", produced by Kitware. VTK provides a great deal of functionality to manipulate and visualize data that is useful for finite element model generation and analysis. vtkn88 is a collection of custom VTK classes that extend VTK to add finite element pre-processing functionality. The vtkn88 library objects combined with generic VTK objects can be quickly assembled into pipelines to produce nearly infinite customizability for finite element model generation and post-processing analysis.

Basing vtkn88 on VTK provides the following advantages.

### Large existing library of objects and filters

VTK is a large and well established system, with many useful algorithms already packaged as VTK objects.

#### **Built-in visualization**

VTK was designed for rendering medical data. With it sophisticated visualizations are readily obtained. The visualization application ParaView is built with VTK and provides excellent complex data visualization. vtkn88 functionality is easily incorporated into ParaView.

#### Standardization

The time and effort the user invests in learning vtkn88 provides familiarity with the widely-used VTK system, and is not limited in application to Numerics88 software.

#### Extensibility

The advanced user is able to write their own VTK classes where required.

### **Multiple Language Support**

VTK itself consists of C++ classes, but provides wrapping functionality to generate an interface layer to other languages. vtkn88 uses this wrapping functionality to provide a Python interface.

The best way to learn to use vtkn88 is to follow the tutorials in Chapter 7.

### Tip

We recommend that you use Python for assembling programs with vtkn88. There are several advantages of using Python, including simplicity of syntax and automatic memory management. In our experience, writing programs using vtkn88 in Python is far less time consuming, and results in programs that are much easier to debug than writing the same programs in C\++. This is particularly true for users without significant programming experience.

### Тір

Many of the tools provided with Faim are implemented as Python scripts. Some use vtkn88, and some manipulate the n88model file directly through netcdf4-python, which is included in the Faim distribution. Examining how they work can be a good way to learn how to write your own custom python scripts for manipulating Faim data. You can find the scripts in the tools directory of your distribution.

### 3.1 vtkn88 API documentation

The complete Application Programming Interface (API) reference documentation for vtkn88 is provided in your installation directory in HTML format at doc/vtkn88/html/index.html. It can be read with any browser. This document is hyperlinked to the vtkn88 API documentation, so that if you click on a class name, it should open the documentation for that class in a browser. There are a few caveats however; the hyperlinking only works if the documentation (including this file) is in the original installation locations. Furthermore, Apple's Preview doesn't support hyperlinking from PDFs to the local file system for security reasons. We recommend using Adobe PDF reader instead.

The API documentation gives complete details of the C++ interface of every class in vtkn88. You should refer to the vtkn88 API reference documentation whenever using a vtkn88 class, as the descriptions below are introductory, and do not exhaustively cover all the functionality.

API documentation for VTK itself can be found at http://www.vtk.org/doc/release/5.10/html/.

### Note

If you are using Python instead of C++ (and for most purposes, we recommend that you do), then you will have to infer the Python interface from the C++ interface. This is generally simple: class and method names are the same, as are all positional argument names. Since Python is a weakly-typed language, you do not need to be concerned generally with the declared type of the arguments. A small number of C++ methods in vtkn88 do not have a Python equivalent, but this is rare.

### 3.2 Array indexing in vtkn88

Arrays in vtkn88, as in VTK, C and Python, are zero-indexed. That is, the first element is element 0. This applies also to node numbers and element numbers. (It does not however apply to material IDs, because the material ID is not an array index; it is a key into a table look-up.) Be careful if reading an n88model file directly, because node numbers and element numbers are stored 1-indexed (see the file specification). The translation is done automatically if you use the vtkn88 objects vtkn88N88ModelReader and vtkn88N88ModelWriter.

### 3.3 Typical workflow for vtkn88

Figure Figure 3.1 shows a typical work flow for creating a finite element model using vtkn88. VTK generally consists of two types of objects (or "classes"): objects that contain data, and objects that process data. The latter are called "filters". Filters can be chained together to create a processing pipeline. In the figure, filters are listed in the boxes with dark black lines and rounded corners; data objects are listed in gray rectangles. The boxes with dark black lines and rounded corners represent actions, and may list one or more VTK or vtkn88 objects that are suitable for performing the action.



The typical way to use a VTK filter object is to create it, set parameters, set the input (if relevant), call Update(), and then get the output. For example, for a vtkn88AIMReader object, which has an output but no input, we might do this in Python

```
reader = vtkn88.vtkn88AIMReader()
reader.SetFileName ("MYFILE.AIM")
reader.Update()
image = reader.GetOutput()
```

### Тір

There is an alternate way to use VTK filter objects, and that is to chain them together in a pipeline. In this case, calling Update on the last item in the pipeline will cause an update of all the items in the pipeline, if required. To connect filters in a processing pipeline, use SetInputConnection and GetOutputPort instead of SetInputData and GetOutput. As an example, we can connect a vtkn88AIMReader to a vtkn88ImageToMesh like this

This automatically calls Update on the reader. Generally, unless you have some application where the pipeline approach is advantageous, we recommend the simpler method of using SetInputData and GetOutput and explicitly passing the data object between filters.

### 3.4 The vtkn88FiniteElementModel object

The central class that vtkn88 adds to VTK is a new type of data class, called vtkn88FiniteElementModel . The conceptual structure of vtkn88FiniteElementModel is shown in Figure 3.2. vtkn88FiniteElementModel is a subclass of the VTK class vtkUnstructuredGrid , which represents a data set as consisting of an assortment of geometric shapes. In VTK terminology, these individual shapes are "Cells". They map naturally to the concept of Elements in finite element analysis. The vertices of the cells, in VTK terminology, are "Points". These are equivalent to Nodes in finite element analysis. vtkUnstructuredGrid , like other VTK objects, is capable of storing specific types of additional information, such as one or more scalar or vector values associated with each Cell or Point. This aspect is used for storing, for example, material IDs, which are mapped to the scalar values of the Cells. To vtkUnstructuredGrid , vtkn88FiniteElementModel adds some additional information related to requirements for finite element analysis such as material properties and constraints (*i.e.* displacement boundary conditions and applied loads), as well as sets of Points and/or Cells, which are useful for defining constraints and in post-processing. Sets and constraints are indexed by an assigned name, which is convenient for accessing and modifying them.



Figure 3.2: Structure of vtkn88FiniteElementModel.

### 3.5 Reading a segmented image

We typically read in data as a segmented 3D volumetric image from micro-CT. The image values (*i.e.* the pixel or voxel values) need to correspond to the segmented material IDs. The selection of a file reading object will be appropriate to the input file format. The output of the file reader filter will be a vtkImageData object.

We have already given the example of using a vtkn88AIMReader to read a Scanco AIM file, which was

```
reader = vtkn88.vtkn88AIMReader()
reader.SetFileName ("MYFILE.AIM")
reader.Update()
image = reader.GetOutput()
```

#### Important

One slightly obscure technical issue which may arise is: are the data of a vtkImage associated with the Points or the Cells? Either is possible in VTK. The scalar image data (scalar because there is one value per location) must be explicitly associated either with the Cells or with the Points. (In fact it's possible to have different scalar data on the Cells and the Points.) Thinking about it as an FE problem, it is natural to associate the image data with Cells, where each image voxel becomes an FE element. Thus, we like to think of each value in the image as being at the center of a Cell in the VTK scheme. VTK however has generally standardized on the convention of image data being on the Points. There are some important consequences. For example, a vtkImage that has dimensions of (M,N,P) has (M,N,P) Points, but only (M-1,N-1,P-1) Cells. Or conversely, if you have data with dimensions of (R,S,T), and you want to put the data on the Cells, then you actually require a vtkImage with dimensions of (R+1,S+1,T+1). Also, if the origin is important, one needs to keep in mind that the origin is the location of the zero-indexed Point. In terms of the Cells, this is the "lower-left" corner of the zero-indexed Cell, not the center of that Cell. vtkn88 objects that require images as input will accept input with data either on the points or on the Cells. However, many VTK objects that process images work correctly only with input data on the Points. By contrast, if you want to render the data and color according to the scalar image, the rendering is quite different depending on whether the scalar data is on the Points or the Cells. Generally, you get the expected result in this case by putting the data on the Cells. This discussion is important because it illustrates that there is no one universally correct answer to whether image data belongs on the Points or on the Cells. vtkn88 image readers, such as vtkn88AIMReader have an option DataOnCells to control the desired behaviour. VTK image readers always put image data on the Points, so if you need the data on the Cells, you must to copy the output to a new vtklmage.

Examples of reading data with vtkn88 are given in the tutorials Compressing a cube revisited using vtkn88 and Advanced custom model tutorial: a screw pull-out test.

### 3.6 Reading an unsegmented image and segmenting it

If you have an unsegmented image such as a raw micro-CT image that has scalar values still in terms of density, it is possible to process the image with VTK. Segmentation is a complex subject, which we are unable to cover here. For an example of a simple segmentation, where only a density threshold and connectivity are considered, consult the example in the directory examples/segment\_dicom.

### 3.7 Ensuring connectivity

A well-defined problem for finite element analysis requires that all parts of the object in the image be connected as a single object.

Disconnected parts in the input create an ill-defined problem, with an infinite number of solutions. These arise, for example, when there is noise in the image data. Some solvers cannot solve this kind of problem at all (the global stiffness matrix is singular). n88solver will typically find a solution. However, the convergence might be very slow as it attempts to find the non-existent optimum position for the disconnected part.

To avoid this problem, the input image can be processed with the filter ImageConnectivityFilter. This filter has many options and different modes of operation, but in most cases the default mode is sufficient. In the default behaviour:

- 1. Zero-valued voxels are considered "empty space", and no connection is possible though them.
- 2. Voxels are considered connected if they share a face. Sharing only a corner or an edge is not sufficient.
- 3. Only the largest connected object in the input image is passed to the output image. Smaller objects that have no continuous path of connection to the largest connected object are zeroed-out.

Because of the first point, it is clearly necessary to segment the image before applying ImageConnectivityFilter, because empty space must be labelled with the value 0.

```
connectivity_filter = vtkn88.vtkn88ImageConnectivityFilter()
connectivity_filter.SetInput (image)
connectivity_filter.Update()
image = connectivity_filter.GetOutput() •
```

**1**, **1** Notice that we use the variable name "image" for both the input and the output. This causes no problems in Python, although by doing this we can no longer use this to refer to the input image. If that were necessary, then we should use different names for the input and output.

If your input image is processed and segmented with another software package, it is still a good idea to verify the connectivity of the input image. If your input image is carefully prepared, and you don't want to inadvertently modify it, you can check for connectivity without modifying it like this:

```
connectivity_mapper = vtkn88.vtkn88ImageConnectivityMap()
connectivity_mapper.SetInput (image)
connectivity_mapper.Update()
if connectivity_mapper.GetNumberOfRegions() != 1:
    print "WARNING: Input image does not consist of a single connected object."
```

Examples of ensuring connectivity are given in the tutorials Compressing a cube revisited using vtkn88 and Advanced custom model tutorial: a screw pull-out test.

### 3.8 Generating a mesh

Once we have a segmented and connected image, we convert the image to a mesh of elements, represented by a vtkUnstructuredGrid object. The base class vtkUnstructuredGrid supports many types of Cells, but currently vtkn88 supports only VTK\_-HEXAHEDRON and VTK\_VOXEL. The topology of VTK\_VOXEL is shown in Figure 3.3.



Figure 3.3: Topology of VTK\_VOXEL. Local numbering of the nodes (Points) of the element (Cell) is shown (0-indexed).

Generating a mesh in vtkn88 is straightforward; simply pass the input image to a vtkn88ImageToMesh filter. It takes no options; the important choices were made already during the segmentation stage. In Python this looks like this

```
mesher = vtkn88.vtkn88ImageToMesh()
mesher.SetInput (image)
mesher.Update()
mesh = mesher.GetOutput()
```

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vtkn88ImageToMesh creates one Cell (*i.e.* element) of type VTK\_VOXEL for every voxel in the input image that has non-zero scalar value. The scalar values of the image become the scalar values of the output Cells. It also creates Points at the vertices (corners) of the Cells. There are no duplicate Points: neighbouring Cells will reference the same Point on shared vertices.



#### Important

Cells and Points in VTK are ordered; they can be indexed by consecutive Cell or Point number. This ordering is not inconsequential. In Faim, the solver efficiency is optimal with certain orderings, and in fact there are orderings for which the solver fails with an error message. The ordering output by vtkn88ImageToMesh is "x fastest, z slowest". It is recommended to always preserve this ordering.

### 3.9 Defining materials

Material definitions are generated by creating a instance of a class of the corresponding material type, and then calling the appropriate methods to set the material parameters. Every material must have a unique name. vtkn88 will assign default unique names when defining a new material object, but the names will be more meaningful if you assign them yourself.

vtkn88 7.0 supports the following material classes:

- vtkn88LinearIsotropicMaterial
- vktn88LinearOrthotropicMaterial
- vktn88LinearAnisotropicMaterial
- vtkn88VonMisesIsotropicMaterial
- vtkn88MohrCoulombIsotropicMaterial

Here is an example of creating a simple linear isotropic material:

```
linear_material = vtkn88.vtkn88LinearIsotropicMaterial()
linear_material.SetYoungsModulus (800) ①
linear_material.SetPoissonsRatio (0.33)
linear_material.SetName ("Linear 800")
```

• As discussed in A note about units, the units of Young's modulus depend on the input length units. If the length units are mm and force units in N, then Young's modulus has units of MPa.

This is the construction of a Mohr-Coulomb elastoplastic material:

```
ep_material = vtkn88.vtkn88MohrCoulombIsotropicMaterial()
ep_material.SetYoungsModulus (800)
ep_material.SetPoissonsRatio (0.33)
ep_material.SetYieldStrengths (20, 40) •
ep_material.SetName ("Mohr Coulomb material 1")
```

• For Mohr-Coulomb, this pair of numbers is the yield strength in tension and the yield strength in compression. The units of yield strength are the same as stress, so typically MPa.

### 3.10 Constructing a material table

Once you have created your material definitions, you need to combine them into a material table, which maps material IDs to the material definitions.

For example, if we want a homogenous material, and the input image has only the scalar value 127 for bone (and 0 for background), then we can make a material table like this:

```
materialTable = vtkn88.vtkn88MaterialTable()
materialTable.AddMaterial (127, linear_material) ①
```

• We created the material linear\_material above.

We must assign a material for every segmentation value present in the input. The same material can be assigned to multiple material IDs. For example, suppose the input image has segmentation values 100-103, and we have created two different materials, materialA and materialB, then we could create a vtkn88MaterialTable like this:

```
materialTable = vtkn88.vtkn88MaterialTable()
materialTable.AddMaterial (100, materialA)
materialTable.AddMaterial (101, materialB)
materialTable.AddMaterial (102, materialB)
materialTable.AddMaterial (103, materialB)
```

There are a couple of helper classes that simplify the creation of material tables for common cases. For a model with a homogenous material, we can use vtkn88GenerateHomogeneousMaterialTable. This class assigns a specified vtkn88Material to all the scalar values present in the input. The size of the resulting material table depends on the number of distinct input values. For example,

```
mtGenerator = vtkn88.vtkn88GenerateHomogeneousMaterialTable()
mtGenerator.SetMaterial (material1)
mtGenerator.SetMaterialIdList (mesh.GetCellData().GetScalars())
mtGenerator.Update()
materialTable = mtGenerator.GetOutput()
```

We could alternatively set SetMaterialIdList with the scalars from the image, rather than those of the mesh; the results will be the same.

Another useful helper class is vtkn88GenerateHommingaMaterialTable . Refer to the section on the Homminga material model in the chapter on preparing models with n88modelgenerator.

Examples of defining materials and creating a material table are given in the tutorials Compressing a cube revisited using vtkn88, Deflection of a cantilevered beam: adding custom boundary conditions and loads and Advanced custom model tutorial: a screw pull-out test.

### 3.11 Creating a finite element model

At this stage, we combine the geometric mesh with the material table to create a vtkn88FiniteElementModel object. The most elementary way to do this is with a vtkn88FiniteElementModelGenerator, which can be used like this

```
modelGenerator = vtkn88.vtkn88FiniteElementModelGenerator()
modelGenerator.SetInput (0, mesh)
modelGenerator.SetInput (1, materialTable)
modelGenerator.Update()
model = modelGenerator.GetOutput()
```

After combining the mesh with the material table, all that is now required to make a complete finite element model is to add boundary conditions and/or applied loads, and to specify node and element sets for the post-processing. For standard tests, there are vtkn88 filters to generate complete models, and these are described below in Section 3.17.

### 3.12 Creating node and element sets

Before we can create boundary conditions or applied loads, we need to define node and/or element sets that specify all the nodes (or elements) to which we want to apply the boundary condition (displacement or applied load). Node and element sets are also used during post-processing. This will be discussed later in Setting post processing parameters.

Any number of node and element sets may be defined. They must be named, and they are accessed by name. The node and element sets are simply lists of node or element numbers, and are stored as vtkIdTypeArray. There are many ways to create node and element sets. A very simple way is to simply enumerate the node numbers (or element numbers). For example, if we wanted to create a node set of the nodes 8,9,10,11, this would be the code:

```
nodes = array ([8,9,10,11])
nodes_vtk = numpy_to_vtk (nodes, deep=1, array_type=vtk.VTK_ID_TYPE) 
nodes_vtk.SetName ("example_node_set")
model.AddNodeSet (nodes_vtk)
```

In Python, the most flexible way to handle array data is with numpy arrays, however the data must be passed to VTK objects as vtkDataArray.numpy\_to\_vtk does the conversion.

VTK offers many ways to select Points and Cells, for example by geometric criteria. As an example of this, refer to the screw\_pullout\_tutorial where a node set is selected from nodes located on a particular rough surface, and subject to additional criterion  $r_1 < r < r_2$ , where *r* is the radius from a screw axis.

vtkn88 also offers some utility functions for identifying node and elements sets. These can be found in vtkn88SelectionUtilities

Frequently, we require sets corresponding to the faces of the model (*i.e.* the boundaries of the image). In this case, we may use the class vtkn88ApplyTestBase . vtkn88ApplyTestBase is a subclass of vtkn88FiniteElementModelGenerator , with the extra functionality of creating pre-defined sets. vtkn88ApplyTestBase implements the concept of a Test Frame and a Data Frame. Refer to test orientation in the chapter on n88modelgenerator. vtkn88ApplyTestBase creates the node and element sets given in the following table. Note that in each case there is both a node and element set, with the same name.

Table 3.1: Node and element s	ets generated by vtkn88ApplyTestBase

Set name	Consists of
face_z0	nodes/elements on the bottom surface $(z=z_{min})$ in the Test Frame.
face_z1	nodes/elements on the top surface $(z=z_{max})$ in the Test Frame.
face_x0	nodes/elements on the $x=x_{min}$ surface in Test Frame.
face_x1	nodes/elements on the $x=x_{max}$ surface in Test Frame.
face_y0	nodes/elements on the $y=y_{min}$ surface in Test Frame.
face_y1	nodes/elements on the $y=y_{max}$ surface in Test Frame.

The sets "face\_z0" and "face\_z1" are of particular importance, as the standard tests are applied along the z axis in the Test Frame.

vtkn88ApplyTestBase has options UnevenTopSurface() and UnevenBottomSurface() by which we can choose to have "face\_z0" and/or "face\_z1" as the set of nodes/elements on an uneven surface, instead of the boundary of the model. This is especially useful when the object in the image does not intersect the top/bottom boundaries of the image. See further discussion on uneven surfaces in the chapter on n88modelgenerator. The two sets "face\_z0" and "face\_z1" can also be limited to a specific material, as defined by material ID.

vtkn88ApplyTestBase is used identically to vtkn88FiniteElementModelGenerator, except that additional optional settings may be set if desired. For example, here we define a model with a test axis in the *y* direction, and specify that we want the set "face\_z1" to be the uneven surface in the image, where we are limiting the search for the uneven surface to a maximum distance of 0.5 from the image boundary.

```
modelGenerator = vtkn88.vtkn88ApplyTestBase()
modelGenerator.SetInput (0, mesh)
modelGenerator.SetInput (1, materialTable)
modelGenerator.SetTestAxis (vtkn88.vtkn88ApplyTestBase.TEST_AXIS_Y)
modelGenerator.UnevenTopSurfaceOn()
modelGenerator.UseTopSurfaceMaximumDepthOn()
modelGenerator.SetTopSurfaceMaximumDepth (0.5)
```
```
modelGenerator.Update()
model = modelGenerator.GetOutput()
```

An example of using the standard node and element sets from vtkn88ApplyTestBase is given in Deflection of a cantilevered beam: adding custom boundary conditions and loads. The tutorial Advanced custom model tutorial: a screw pull-out test demonstrates a sophisticated selection of custom node sets.

# 3.13 Adding boundary conditions

Once we have created the node sets, creating a boundary condition applied to the nodes of a particular node set is straightforward and can be done with the method ApplyBoundaryCondition() of vtkn88FiniteElementModel. For example, to fix the bottom nodes and apply a displacement of 0.1 to the top nodes, we could do this

```
model.ApplyBoundaryCondition (
    "face_z0",
    vtkn88.vtkn88Constraint.SENSE_Z,
    0,
    "bottom_fixed") ③
model.ApplyBoundaryCondition (
    "face_z1",
    vtkn88.vtkn88Constraint.SENSE_Z,
    -0.1, ③
    "bottom_fixed")
```

- vtkn88.vtkn88Constraint.SENSE\_Z has the value 2 (see vtkn88Constraint). It is possible just to use that value 2 here, but SENSE\_Z is more informative.
- <sup>2</sup> This is the user-defined name assigned to the boundary condition. Every constraint must have a unique name.
- Negative if we want compression.

The "sense" is the axis direction along which the displacement is applied. The other axis directions remain free unless you also specify a value for them. It is quite possible, and common, to call ApplyBoundaryCondition() three times on the same node set, once for each sense.

ApplyBoundaryCondition() can take different types of arguments, for example arrays of senses, displacements and node numbers. Refer to the API documentation for vtkn88FiniteElementModel. There is also a convenience method FixNodes(), which is a quick way to set all senses to a zero displacement.

Boundary conditions are implemented within vtkn88FiniteElementModel as a specific type of vtkn88Constraint . All the constraints associated with a vtkn88FiniteElementModel are contained in a vtkn88ConstraintCollection . It is possible to modify either vtkn88ConstraintCollection or a particular vtkn88Constraint manually. For example, we could create a boundary condition on two nodes in the following manner. This is somewhat laborious and usually unnecessary, but it can be adapted to create unusual boundary conditions.

```
node_ids = array([3,5])
node_ids_vtk = numpy_to_vtk (node_ids, deep=1, array_type=vtk.VTK_ID_TYPE)
senses = array ([0,2])  # x-axis, z-axis
senses_vtk = numpy_to_vtk (senses, deep=1, array_type=vtk.VTK_ID_TYPE)
senses_vtk.SetName ("SENSE")
values = array([0.1,0.1])
values_vtk = numpy_to_vtk (values, deep=1, array_type=vtk.VTK_ID_TYPE)
values_vtk.SetName ("VALUE")
constraint = vtkn88.vtkn88Constraint()
constraint.SetName ("a_custom_boundary_condition")
constraint.SetIndices (node_ids)
constraint.SetConstraintType (vtkn88.vtkn88Constraint::DISPLACEMENT)
constraint.SetConstraintAppliedTo (vtkn88.vtkn88Constraint::NODES)
```

```
constraint.GetAttributes().AddArray (senses)
constraint.GetAttributes().AddArray (values)
model.GetConstraints().AddItem (constraint)
```

Examples of applying boundary conditions are given in the tutorials Deflection of a cantilevered beam: adding custom boundary conditions and loads and Advanced custom model tutorial: a screw pull-out test.

# 3.14 Adding applied loads

Creating an applied load is similar to creating a displacement boundary condition. They are both implemented as vtkn88Constraint . However, while displacement boundary conditions are applied to nodes, applied loads are applied to elements; in fact they are applied to a particular face of an element (or to the body of an element). Therefore, the ApplyLoad() method of vtkn88FiniteElementModel takes the name of an element set, and has an additional input argument which specifies to which faces of the elements the load is applied. Here is an example of creating an applied load on the top surface of the model:

```
model.ApplyLoad (
    "face_z1", ①
    vtkn88.vtkn88Constraint.FACE_Z1_DISTRIBUTION,
    vtkn88.vtkn88Constraint.SENSE_Z, ②
    6900, ③
    "bottom_fixed")
```

- Refers to the element set "face\_z1", not the corresponding node set, which very often also exists with the same name.
- In this example, the applied force is perpendicular to the specified element face, but it is not required to be so.
- This is the total load applied. The load is evenly distributed between all of the element faces.

To apply forces along non-axis directions, call ApplyLoad () multiple times with different senses.

As with displacement boundary conditions, we can create an applied force manually, if we require more flexibility. It will look something like this:

```
element_ids = array([3, 5])
element_ids_vtk = numpy_to_vtk (element_ids, deep=1, array_type=vtk.VTK_ID_TYPE)
distributions = ones ((2,)) * vtkn88.vtkn88Constraint.FACE_Z1_DISTRIBUTION
distributions_vtk = numpy_to_vtk (distributions, deep=1, array_type=vtk.VTK_ID_TYPE)
distributions_vtk.SetName ("DISTRIBUTION")
                          # x-axis, z-axis
senses = array ([0,2])
senses_vtk = numpy_to_vtk (senses, deep=1, array_type=vtk.VTK_ID_TYPE)
senses_vtk.SetName ("SENSE")
total load = 6900
values = total_load * ones(2, float) / 2
values_vtk = numpy_to_vtk (values, deep=1, array_type=vtk.VTK_ID_TYPE)
values vtk.SetName ("VALUE")
constraint = vtkn88.vtkn88Constraint()
constraint.SetName ("a_custom_applid_load")
constraint.SetIndices (element_ids)
constraint.SetConstraintType (vtkn88.vtkn88Constraint::FORCE)
constraint.SetConstraintAppliedTo (vtkn88.vtkn88Constraint::ELEMENTS)
constraint.GetAttributes().AddArray (distributions)
constraint.GetAttributes().AddArray (senses)
constraint.GetAttributes().AddArray (values)
model.GetConstraints().AddItem (constraint)
```

### Тір

You can apply loads to nodes instead of to elements if you desire. You must create a constraint by hand to do this, as there is no convenience method provided for this purpose. This is most sensible when you desire to apply a point force (*i.e.* to a single node). Be careful about applying forces to nodes because applying a constant force to each of a set of nodes on a surface is *not* equivalent to applying a uniform pressure to that surface. By contrast, applying a constant force to a set of element faces is equivalent to a uniform pressure, which is why it is usually more convenient to define loads on element faces.

#### Important

Applied loads are additive. That is, if you create more than one applied load on a particular element face, the loads will add. Displacement boundary conditions by contrast are unique. If you create more than one displacement boundary condition applying to a particular node and sense, then only one of them will be used by the solver, and the other will be discarded. Which of multiple boundary conditions applying to the same degree of freedom is used is indeterminate, so it is a logical error to create multiple different boundary conditions applying to the same degree of freedom. No warning or error message will be generated in the case of multiple boundary conditions on the same degree of freedom. (It is sometimes convenient to be able to do so in cases where the actual value used turns out not to matter).

An example of adding an applied load is given in the tutorial Deflection of a cantilevered beam: adding custom boundary conditions and loads.

# 3.15 Ensuring your model is well-defined

It is possible to create a model that is degenerate, or not well-defined. In other words, a model that has not a single solution, but many solutions (typically an infinite number). As a linear algebra problem, such a problem has a singular global stiffness matrix. For example, consider the standard uniaxial problem where a sample volume is compressed between two hard parallel plates. (See uniaxial test in the chapter on n88modelgenerator). If we specify no contact friction, then although the sample compresses in a predictable way between the two plates, it is free to slide around as a whole (translate) anywhere between the plates. For the particular case of the uniaxial model, n88modelgenerator provides the option to add a pin, which consists of the following additional constraints:

- 1. fix the *x*,*y* senses of an arbitrary node, and
- 2. fix one sense of another node (usually from the same element).

The first constraint is sufficient to prevent translation, and the second constraint is required to prevent rotation.

Models with only applied loads and no displacement boundary conditions are always ill-defined.

Practically, n88solver will usually solve even ill-defined problems. In fact, for the type of ill-defined problem described here, it often does so faster than the equivalent well-defined problem (*i.e.* one with added "pin" constraints to make it non-singular). Many types of ill-defined problems can cause n88solver to converge much more slowly. For example, see the discussion on Ensuring connectivity. Not all solvers however can handle ill-defined problems, so this should be avoided when exporting models to other solvers. Also, if you would like overlay the renderings of two similar ill-defined problems or compare differences in any way, it is usually necessary to first register them to eliminate meaningless differences (such as overall translations or rotations in the example described).

# 3.16 Setting post-processing parameters

If you have followed every step, then you have a model that is completely defined for the solver. In fact you could save it to a file and solve it now. The post-processor n88postfaim however requires a bit more information so that meaningful results can be extracted from the solved model. n88postfaim calculates certain quantities with reference to node or element sets. For example, in a compression test the relevant sets correspond to the top and bottom faces, as we are interested principally in the forces on these faces. These sets already exist ("face\_z0" and "face\_z1"), as we previously used them to apply boundary conditions. We

need to list the relevant node sets to be used by n88postfaim. Of course, if you're doing some custom post-processing that does not involve n88postfaim, then this step is optional and can be skipped. Setting the post-processing node sets involves setting some "information" with a key (this may seem slightly obscure, but it is a standard VTK technique):

```
info = model.GetInformation()
pp_node_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_NODE_SETS()
pp_node_sets_key.Append (info, "face_z0")
pp_node_sets_key.Append (info, "face_z1")
```

Any number of sets may be specified for post-processing. n88postfaim requires the element sets as well as the node sets, and they must match exactly, meaning that the  $n^{th}$  post-processing element set must be exactly those elements which contain any of the nodes of the  $n^{th}$  post-processing node set. (The element set name is not required to be the same as the node set name).

If you've used vtkn88ApplyTestBase to get pre-defined node and element sets, then you already have the corresponding element sets, and in fact they have the same names, so

```
info = model.GetInformation()
pp_node_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_NODE_SETS()
pp_node_sets_key.Append (info, "face_z0")
pp_elem_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_ELEMENT_SETS()
pp_element_sets_key.Append (info, "face_z0")
pp_element_sets_key.Append (info, "face_z1")
```

If you've created custom node sets, then you can obtain the corresponding element sets with the method GetAssociatedEl ementsFromNodeSet(), so for example (taken from the screw pull-out tutorial),

```
info = model.GetInformation()
pp_node_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_NODE_SETS()
pp_elem_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_ELEMENT_SETS()
for setname in ["bone_top_visible", "screw_top"]:
    pp_node_sets_key.Append (info, setname)
    elementSet = model.GetAssociatedElementsFromNodeSet (setname)
    model.AddElementSet (elementSet)
    pp_elem_sets_key.Append (info, setname)
```

Examples of setting post-processing parameters are given in the tutorials Deflection of a cantilevered beam: adding custom boundary conditions and loads and Advanced custom model tutorial: a screw pull-out test.

# 3.17 Filters for creating standard tests

For each of the standard tests, meaning the ones that n88modelgenerator can generate, there is a filter to generate the test, complete with all displacement boundary conditions, applied forces, and relevant post-processing sets. Of course, it is easier to just simply use n88modelgenerator for these cases rather than write a script. However, these filters provide more options than are exposed by n88modelgenerator, and a script will allow you to access these options. Furthermore, sometimes a standard model is nearly, but not quite, what you want. In this case, the fastest way to proceed is to use a standard test generating filter, and then tweak the resulting model.

All the standard test filters are subclasses of vtkn88ApplyTestBase (see Creating node and element sets), so that they support variable orientation as defined by the Data Frame and the Test Frame, as well as having the standard sets defined ("face\_z0", etc...)

The following table lists the standard model filters.

 Table 3.2: vtkn88 filter classes that generate standard models

vtkn88 filter	n88modelgenerator test types
vtkn88ApplyCompressionTest	uniaxial, axial and confined
vtkn88ApplySymmetricShearTest	symshear

vtkn88 filter	n88modelgenerator test types
vtkn88ApplyDirectionalShearTest	dshear
vtkn88ApplyBendingTest	bending
vtkn88ApplyTorsionTest	torsion

For details on the options supported by these filters, refer to the API documentation.

An example of using a standard test filter is given in the tutorial Compressing a cube revisited using vtkn88.

# 3.18 Modifying a finite element model

Often a standard model type will be very close to the desired test configuration, but some modifications are needed. Every part of vtkn88FiniteElementModel can be modified, or even deleted, after creation. There are in general too many possibilities to enumerate here.

If a model is already written as an n88model file, it can be read with vtkn88N88ModelReader, modified, and rewritten.

# 3.19 Updating the history and the log

It is good practice (but not strictly necessary) to add relevant details to the History and Log fields of a model before writing it out. This will assist greatly in the future if it is required to trace back the origins and history of a given n88model file.

The history and comments of an n88model file can be viewed with the command

n88modelinfo --history --comments myfile.n88model

You can leave out the --history and --comments arguments, although then you will get a lot more information about the model, possibly more than you want.

The History field should have one line per executable that modifies the model file. This line should start with a time/date stamp and briefly state the program (and perhaps the user) which modified or created the file. History can be added with the method AppendHistory(); the date/time stamp will be automatically added. For example

model.AppendHistory("Created with screwpullout.py version 6.0")

The Log field is intended to record any other information that would be useful to be able to recover at a later time. Every addition can be any number of lines long. You should record any parameters or settings that are relevant here. As for AppendHistor y(), AppendLog() will add a date/time stamp (although on its own line). It will also ensure that every addition to the Log is separated by black line from other additions to Log, for ease in reading it. For example

```
settingsText = ["Configuration:",
    "input file
                                    = %s" % input_image_file,
    "output file
                                    = %s" % output_faim_file,
                                    = %s" % bone_material_id,
    "bone material id
    "bone material Young's modulus = %s" % bone_material_modulus,
    "bone material Poisson's ratio = %s" % bone_material_poissons_ratio,
                                    = %s" % screw_material_id,
    "screw material id
    "screw material Young's modulus = %s" % screw_material_modulus,
    "screw material Poisson's ratio = %s" % screw_material_poissons_ratio,
                                   = %s" % screw_displacement,
    "screw displacement
                                   = %s" % inner_ring_radius,
    "inner ring radius
                                  = %s" % bone_constraint_max_depth]
    "bone constraint max depth
```

model.AppendLog ("\n".join(settingsText)) 0

This might look pretty weird if you're not a Python guru. settingsText is a Python list of strings (each of one line).
 "\n".join (settingsText) joins them all into one long string, separated by line returns.

### Тір

A particularly clever trick if your script uses a configuration file to set values, one which is used by n88modelgenerator, and also used in the above example (which is from the screw pull-out tutorial), is to write the settings into the Comment field in exactly the same format that they appear in the configuration file. Then, if ever the data need to be exactly re-created for some reason, the settings can be copied from the Log and pasted directly into a new configuration file. The script can then be rerun with that configuration file without any further editing.

Examples of adding information to the history and to the log are given in the tutorials Compressing a cube revisited using vtkn88, Deflection of a cantilevered beam: adding custom boundary conditions and loads and Advanced custom model tutorial: a screw pull-out test.

# 3.20 Writing a model file for input to the solver

When your vtkn88FiniteElementModel is the way you like it, writing a file is straightforward:

```
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInput (model)
writer.SetFileName ("a_snazzy_model.n88model")
writer.Update()
```

Other formats can also be written using the appropriate writer including,

- vtkn88FaimVersion5InputWriter, and
- vtkn88AbaqusInputWriter .

# 3.21 Visualizing intermediate results

When developing a complicated model, it is often a good idea to write out intermediate results that can be visualized. This can be done either by writing out intermediate geometries and node sets using standard VTK file format writers, such as vtkXMLUnstructuredGridWriter and vtkXMLPolyDataWriter, or by writing the model with vtkn88N88ModelWriter as early as possible as you build up your script, before the model is complete. Even incomplete models can be visualized. The tool n88extractsets is handy to extract and visualize node and element sets, as well as boundary conditions and applied loads.

For an example of visualizing intermediate results as the model is built up, see Advanced custom model tutorial: a screw pull-out test.

# 3.22 Error handling

VTK classes do not throw exceptions or halt execution when an error occurs. If catching error conditions is important to you, you need to provide a VTK observer class. For more information, refer to http://www.vtk.org/Wiki/VTK/Tutorials/Callbacks . However, if you don't provide an error observer (and most often, you won't want to be bothered to), you will still be informed about error conditions by a message printed to standard out (i.e. to the console). For scripting purposes, this is generally adequate.

If you do want to trap the error, here is an example in Python.

```
class ErrorObserver:
    def __init__(self):
        self.__ErrorOccurred = False
        self.__ErrorMessage = None
```

```
self.CallDataType = 'string0'
  def __call__(self, obj, event, message):
      self.__ErrorOccurred = True
      self.__ErrorMessage = message
  def ErrorOccurred(self):
       occ = self.__ErrorOccurred
       self.__ErrorOccurred = False
       return occ
  def ErrorMessage(self):
       return self.__ErrorMessage
errorObserver = ErrorObserver()
reader = vtkn88.vtkn88N88ModelReader()
reader.AddObserver ("ErrorEvent", errorObserver)
reader.SetFileName (filename)
reader.Update()
if errorObserver.ErrorOccurred():
   print "ERROR reading file: ", errorObserver.ErrorMessage()
   sys.exit (-1)
```

vtkn88 provides a very simple error observer class, vtkn88ErrorWarningObserver. Its use however is limited to C\++ code; use the above example for Python.

# **Chapter 4**

# **Solving Linear Problems**

# 4.1 Obtaining solutions to linear problems with n88solver\_sl

For a model with only linear elastic materials, the solver can be run as follows

n88solver\_sl myfile.n88model

The solution as expressed as displacements - from the original position - at node. The displacements are written into the input file; no additional output file is created. If the n88model file contains an existing solution, it will be overwritten. Furthermore, if there is an existing solution, it will be used as a starting point for the solver for further iterations. This behaviour is not always desired and can be suppressed; see restart for details.

#### Tip

To check whether an n88model file has already been solved, the following command is useful

n88modelinfo --history --solutions myfile.n88model

See Section 9.10 for more details.

The complete list of arguments to n88solver is given in the Command Reference chapter.

# 4.2 Convergence

n88solver\_sl is a pre-conditioned conjugate gradient solver which improves the solution through an iterative process. Therefore it is necessary to define a convergence criterion that defines when the solution is good enough, and the iterating can stop.

### **Convergence measure**

n88solver defines a *convergence measure* that can be understood as the degree of change of the solution from one iteration to the next. For the  $i^{th}$  iteration it is defined as

$$e_{i} = \frac{\max_{j} |x_{i,j} - x_{i-1,j}|}{\max_{j} |x_{i,j}|}$$

where  $x_{i,j}$  is the displacement of the  $j^{th}$  degree of freedom at the  $i^{th}$  iteration. The maximum is taken over all degrees of freedom.

The convergence measure is unitless and thus it is straightforward to choose a suitable default convergence value that is somewhat independent of the model. It is also independent of the accuracy of the solution, and typically will continue to decay to smaller values even if the solver reaches a limit where further iterations fail to improve the solution. Such a limit in the accuracy always exists; this property of the convergence measure allows the iterating to stop rather continuing to iterate indefinitely towards an unachievable threshold.

Because  $e_i$  is defined as the maximum over all degrees of freedom, it does not decay smoothly, but can be jumpy or noisy. Relatively large increases from one iteration to the next can be observed. (In contrast, the RMS value would decay smoothly. However we are generally more interested in the question "What is the largest error?" rather than "What is the average error?") A threshold\_window of at least 3 is therefore recommended to ensure that the iterating is not prematurely stopped by a single randomly-obtained low value.

### **Maximum iterations**

In addition to the convergence criterion described above, a *maximum number of iterations* can be set. This is useful for stopping the iterating if the thresholds have been set too low (*i.e.* too strictly). Sometimes we may want to stop and perform a more sophisticated analysis of the quality of the solution before deciding if we want to proceed with further iterations.

Note that no matter how the solver terminated, we can re-launch it, possibly with different convergence criteria. By default, n88solver\_sl will use the existing solution as the starting point and continue to refine it from where it left off.

The run log of n88solver\_sl contains a table of selected values of  $e_i$  and  $r_i$ . You may want to monitor these values as the solver is running to get an idea of how well the solver is converging. It can be informative to plot these on a log-log graph ( $e_i$  and/or  $r_i$  versus *i* or iteration number).

# 4.3 Evaluating solution quality

For a linear problem, the solver is solving a system equivalent to

 $\mathbf{K}\mathbf{x} = \mathbf{f}$ 

where **x** are the displacements, **f** are the forces (including all the internal forces on each node), and **K** is a global stiffness matrix. The solver never actually constructs **K**; the memory requirements would be prohibitive, as **K** is a matrix of size  $N^2$ , where N is the number of degrees of freedom. The residuals are defined as

$$\mathbf{r} = \mathbf{K}\mathbf{x} - \mathbf{f}$$

For the exact solution, the residual vector is identically zero. As we are obtaining a numerical solution rather than an exact solution, we cannot in practice obtain exactly zero-valued residuals. The remaining value of the residuals is a good measure of the accuracy of the solution, with smaller residuals indicating a closer match to the unobtainable perfect solution.

To answer the question, "What is a good value for the residuals?", observe that the residuals have units of force. We therefore need to compare with a characteristic force in the system.

Numerics88 provides a tool, <n88evaluate,n88evaluate>, to evaluate a solution. It is run like this

n88evaluate myfile.n88model

The output related to the residuals looks like this

Analysis of forces (residuals): max err : 3.00E-07 rms err : 3.15E-08 max err/max force : 3.51E-06 rms err/max force : 3.68E-07

The second two numbers are the maximum and RMS residuals, scaled to the maximum nodal force in the solution. These values are a measure of the relative error. Note that this error is only the mathematical error of the solution to the stated system of equations. There are naturally other sources of error, such as that due to the measurement and discretisation of the physical object, and the error in determining the material properties of the object. When the solver is working normally, these other sources of error will be much larger than the remaining mathematical error in the solution obtained by the solver.

n88evaluate also performs a check that the boundary conditions are indeed satisfied:

Analysis of solution displacements at boundary conditions: max err : 0.00E+00 rms err : 0.00E+00

This is a trivial check: anything other zero or very small values indicates a problem with solver.

# **Chapter 5**

# **Solving Nonlinear Problems**

# 5.1 Obtaining solutions to nonlinear problems with n88solver\_sp

If you have defined plasticity for any materials used in your model, then you must use the solver n88solver\_sp, which is a solver suitable for small-strain elastoplastic models. This solver is invoked exactly as is n88solver\_sl. It recognizes a couple of additional options related to the plastic convergence. To solve an elastoplastic model, the solver first obtains a linear elastic solution, and then performs a plastic iteration to update the plastic strain. This is repeated until the plastic convergence criterion is met. Thus linear solutions, consisting of many linear iterations, alternate with single plastic iteration steps.

### Note

It is perfectly possible to run <code>n88solver\_sp</code> on a model with only linear elastic material definitions. <code>n88solver\_sp</code> takes no longer to run on a linear model than does <code>n88solver\_sl</code>. However it does use more memory. Conversely, it is also possible to run <code>n88solver\_sl</code> on a model containing elastoplastic material definitions. In this case, the plasticity is simply ignored, and the linear solution will be obtained.

# 5.2 Obtaining accurate nonlinear solutions by progressively applying loads

In contrast to a linear elastic model, there is in general no single unique solution for a given end-state of a system with elastoplastic characteristics. As discussed in the section plasticity in the chapter *Preparing Finite Element Models with n88modelgenerator*, elastoplastic models exhibit irreversibility and hysteresis, and thus have a path dependence. In other words, a dependence not only on the final state, but on the history in obtaining the final state. For a real object, the history is the time-dependence of the state, presumably starting from some initial neutral state. Within the solver, it is not necessary (or possible) to account for a continuous time dependence of the state: nevertheless even if we solve for a single end state of an elastoplastic model, the solver necessarily traces a path in a mathematical space from some starting point to the final solution. Just as for the real physical situation, this path in mathematical space can affect the final solution. Therefore, the most strictly correct approach to solving nonlinear elastoplastic problems is to incrementally apply loads (or strains), starting with a solution at or near the elastic limit (*i.e.* near the onset of nonlinear behaviour), and obtaining a complete solution, and also more time-consuming. The question is, does this make any practical difference? Frequently, for loads applied monotonically in a single direction, the answer is no. Conversly, if your physical situation involves increasing and decreasing a load, or changing the direction of an applied load, then it is important to model this load history. A tutorial demonstrating the incremental application of a load to an elastoplastic problem is A cantilevered beam with elastoplastic material properties .

# 5.3 Evaluating nonlinear solution quality

Evaluating the correctness of an elastoplastic solution is more subtle than evaluating the correctness of a linear elastic model, for the simple reason that, as mentioned in the previous section, there is no single unique solution to an elastoplastic problem.

There are nevertheless some measures we can use. Internal forces must still balance, and we can examine the residuals, as in Evaluating solution quality in the section on linear models.

When examining the yield strain, there must be no unyielded elements for which a positive yield function is calculated. Here is the check of that in n88evaluate:

```
Analysis of yield function F:

Unyielded elements with F>0:

count : 0

max F : -

rms F : -

max F/max stress : -

rms F/max stress : -
```

Actually in rare cases, a small number of unyielded elements might have very small positive values of yield function, but in this case, the values should be very small indeed.

Secondly, one might expect all the yielded elements in the solution (*i.e.* those elements with a nonzero plastic strain) to lie on the yield surface (F=0). In fact, this is not necessarily the case. Even in an elastoplastic model carefully solved with incremental applied test strain, it may happen that some elements reach the yield stress (*i.e.* the yield surface) for some value of applied test strain, but then actually experience a substantially reduced stress at a higher applied test strain, due to the mechanical failure or yield of some other part of the model. Thus it is perfectly possible to have an end-state solution in which some elements are observed to have non-zero plastic strains but are in a stress state much less than the yield stress (*i.e.* well inside the yield surface). More common though is for yield elements to have a very small remnant positive yield function, which is somewhat analogous to the residual in the linear case.

Values related to the yield function calculated for all yielded elements are reported by n88evaluate, as shown in this example:

```
Analysis of yield function F:
Yielded elements:
count : 2058
min F : -1.85E+01
max F : 1.08E-04
rms F : 7.77E+00
min F/max stress : -2.12E-01
max F/max stress : 1.23E-06
rms F/max stress : 8.88E-02
```

In light of the above discussion, the important value is max F/max stress: it can be used as a measure of the relative error of the plastic component of the solution.

# **Chapter 6**

# **Post-Processing and Analysis**

# 6.1 Calculating additional solution fields with n88derivedfields

The fundamental solution from n88solver are the displacements on each node. However, this is often not the only value of interest. Subsequently running n88derivedfields on the n88model file will generate additional fields and add them to the active solution in the file.

### Тір

To check which solution fields are present in a n88model file, run

n88modelinfo --solutions your\_model.n88model

The following are the additional fields that will be added to the n88model file by n88derivedfields.

### ReactionForce

The reaction force at each node, in the 3 coordinate directions  $(f_x, f_y, f_z)$ . For a linear problem the reaction force is given by

 $\mathbf{f} = \mathbf{K}\mathbf{x}$ 

This is of course the same equation that the solver has solved, except that now we use it with the solution values for  $\mathbf{x}$  (the displacements) to determine forces. If the solution is accurate, then the forces will be nearly all zero, except on degrees of freedom where a boundary condition (displacement or applied force) applies. Those therefore are the interesting values.

### Strain

The strain at each element, given by  $\varepsilon_{xx}$ ,  $\varepsilon_{yy}$ ,  $\varepsilon_{zz}$ ,  $\gamma_{yz}$ ,  $\gamma_{zx}$ ,  $\gamma_{xy}$ , where  $\varepsilon_{ii}$  is the *engineering normal strain* along the axis direction *i*, and the  $\gamma_{ii}$  are the *engineering shear strains*.

Note that the field Strain is always the total strain, so that for elasto-plastic models, the elastic strain can be obtained by subtracting PlasticStrain from Strain.

#### PlasticStrain

The plastic strain at each element. The plastic strain is the irreversible strain that arises from further deformation once the elastic limits as defined by the yield surface as been reached. PlasticStrain has the same 6 components as Strain.

#### Stress

The stress at each element, given by  $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{zx}, \sigma_{xy}$ .

Note that the stress can be obtained directly from the strain (and vice versa) using the material properties. See Elastic material properties.

### VonMisesStress

The von Mises stress is a scalar value that is frequently used as a yield criterion. It is also used as a heuristic measure of the "magnitude" of the stress at a point, for example for the purpose of coloring a rendering according to stress concentration. It is defined on each element by

$$\sigma_{v}^{2} = \frac{1}{2} \left( (\sigma_{xx} - \sigma_{yy})^{2} + (\sigma_{yy} - \sigma_{zz})^{2} + (\sigma_{zz} - \sigma_{xx})^{2} \right) + 3 \left( \sigma_{yz}^{2} + \sigma_{zx}^{2} + \sigma_{xy}^{2} \right)$$

It can also be expressed more concisely as a norm of the devatoric stresses. For details refer to any Mechanics of Solids textbook.

#### StrainEnergyDensity

The strain energy density is given by

$$U = \frac{1}{2} \left( \sigma_{xx} \varepsilon_{xx} + \sigma_{yy} \varepsilon_{yy} + \sigma_{zz} \varepsilon_{zz} + \sigma_{yz} \gamma_{yz} + \sigma_{zx} \gamma_{zx} + \sigma_{xy} \gamma_{xy} \right)$$

This expression continues to be valid even for nonlinear elastoplastic models, provided that the strain values are limited to the elastic strain component.

In a finite element context, the strain energy density is a scalar value defined on each element.

# 6.2 Exporting solution fields from the model file

If n88postfaim, which is described in the next section, provides the values which are of interest to you, you will not need the numerical data of the solution fields. In other cases, where you want do some custom post-processing on the solution, it will be necessary to obtain the solution fields as array data. There are several options for obtaining the field data from an n88model file:

- 1. Use n88extractfields to export fields to a text file. This is convenient because text files are easy to understand and easy to import. The trade off is that text files are inefficient in terms of disk space required, and relatively slow to write and read.
- 2. Use the vtkn88 object vtkn88N88ModelReader . This requires writing some code in C++ or Python.
- 3. Import the data into third party software that can read NetCDF4 or HDF5.

# 6.3 Obtaining standard post-processing values with n88postfaim

n88postfaim is a tool performs a number of standard analyses on a solved n88model file. It produces a text file output reporting summarized results in a table format.

## 6.3.1 Running n88postfaim

n88postfaim requires that n88derivedfields has been run on the solved n88model file because it makes use of the derived fields. If any field is required for a particular table, but is not present in the n88model file, n88postfaim will simply silently skip that table.

In the usual case, running n88postfaim is as simple as,

n88postfaim -o analysis.txt radius\_slice82\_bending.n88model

This will generate an output file analysis.txt. The output is a report of values that are commonly of interest in finite element calculations.

The sections below will discuss a few important options that affect the output of n88postfaim. For a complete list of arguments supported by n88postfaim, see the Command Reference chapter.

#### Note

The model radius\_slice82\_bending.n88model, which is used in examples below, can be generated from the data file radius\_slice82.aim, with the following command:

n88modelgenerator --test=bending radius\_slice82.aim

This data file is provided for the radius compression tutorial, but here we apply a bending test so that angular analysis quantities such as torques are defined. This model also has been segmented to have more than one material ID. In particular, ID 127 is used to identify cortical bone and ID 100 is used to identify cancellous bone.

This applies to all tables except Plastic Strain, for which the flag --plasticity=vonmises, 40 was added to the n88mo delgenerator arguments.

#### 6.3.1.1 Specifying post-processing node and element sets

Some of the quantities that n88postfaim reports are calculated with respect to defined node and/or element sets. For example, for a compression test, the forces on the top and bottom surfaces are of interest. If we define node and element sets corresponding to these surfaces, then n88postfaim will, amongst other things, calculate these forces for us. Post-processing node and element sets must be defined during the model generation stage. If you used n88modelgenerator, some relevant node and element sets have automatically been defined. For custom models generated with vtkn88 see Creating node and element sets.

The available sets in an n88model file can be discovered with n88modelinfo. For example, the command

n88modelinfo --sets --element\_sets radius\_slice82\_bending.n88model

gives the following output:

```
NodeSets:
 Name : face_z0
 Part : Part1
 NumberOfNodes : 40032
 Name : face z1
 Part : Part1
 NumberOfNodes : 25991
 Name : face_x0
 Part : Part1
 NumberOfNodes : 15
 Name : face_x1
 Part : Part1
 NumberOfNodes : 14
 Name : face_y0
 Part : Part1
 NumberOfNodes : 27
 Name : face_y1
 Part : Part1
 NumberOfNodes : 17
ElementSets:
 Name : face_z0
 Part : Part1
  NumberOfElements : 28999
```

Name : face\_z1
Part : Part1
NumberOfElements : 21210
Name : face\_x0
Part : Part1
NumberOfElements : 8
Name : face\_x1
Part : Part1
NumberOfElements : 6
Name : face\_y0
Part : Part1
NumberOfElements : 12
Name : face\_y1
Part : Part1
NumberOfElements : 8

Given that the sets of interest have been generated and are present in the n88model file, we must tell n88postfaim which to actually use. Much of the time this is also done at the model generation stage. For models generated with vtkn88, see Setting post-processing parameters. n88modelgenerator also writes a list of sets to use into the n88model file, but note that this list often does not encompass all of the available sets. For example, for any type of compression test, n88modelgenerator will only list the top and bottom surface sets to be used for post-processing, although it generates node and element sets for all faces. In a confined test the forces on the side faces are sometimes of interest, so this may be a case where the list of post-processing sets as generated by n88modelgenerator is insufficient. n88postfaim has command line options that allow us to override the list of post-processing sets from the n88model file. Here an example:

```
n88postfaim --node_sets face_y0,face_y1 --element_sets face_y0,face_y1 -o analysis.txt ↔ radius_slice82_bending.n88model
```

Note that for each node set, n88postfaim requires the corresponding element set. For example, for a set consisting of all the nodes on a surface, we also require the set of all elements on the surface. n88modelgenerator (and vtkn88 objects which generate sets automatically) will generate sets such that the corresponding node and element sets have the same names. If this is the case, that we have matching node and element sets, then a simpler but equivalent version of the above example command is

n88postfaim --sets face\_y0,face\_y1 -o analysis.txt radius\_slice82\_bending.n88model

#### 6.3.1.2 Specifying a rotation center

Certain quantities, such as rotations and torques, are calculated relative to a reference point, or center. This reference point can be specified in a number of ways:

- 1. For bending and torsion tests, n88modelgenerator will write a default rotation center into the n88model file, which will be located at the center of mass of the model.
- 2. n88modelgenerator supports an argument central\_axis that allows the reference point to be specified, as as numerical coordinates or as the center of mass or the center of bounds. The reference value will be written to the n88model file. If specified, it overrides the above default.
- 3. n88postfaim supports an argument rotation\_center that can be used to specify the reference point. If specified, it overrides any value in the n88model file.

If the rotation point is not specified in one of these ways, then the corresponding analysis values and tables will not be calculated or reported. This simplifies the analysis output for models for which these values are typically not of interest (*e.g.* an axial compression test).

## 6.3.2 Description of output tables

Below are listed the tables provided in the output of n88postfaim.

Note that not all values or tables are generated for every model. Angular values are generated only if a rotation center is defined (see the above section), while a break-down of values per material is only performed in the case that more than one material is defined.

### Important

n88postfaim knows nothing of the Test Frame coordinate system (see Test Orientation). All coordinate directions in the analysis file are in the original Data Frame coordinate system. An exception is that the names of the sets, as assigned by n88modelgenerator and listed in Table 3.1, are obtained from their orientation in the Test Frame.



### ) Important

The table numbering is not fixed. Tables are simply numbered sequentially at the time they are generated. You cannot rely on a certain table number consistently identifying a given table.

### 6.3.2.1 Model Input

This table lists general parameters of the model input.

Table 1: Model Input

Filename:	radius_slice82_bending.n88model
Element dim X:	0.082
Element dim Y:	0.082
Element dim Z:	0.082
Number of elements:	2667590
Number of nodes:	3816642
Number of nodes per element:	8
Dimension of problem:	3

#### 6.3.2.2 Materials

The material definitions as assigned to each material ID are listed. In addition, a very brief summary of the material definition is provided, in particular the material type is shown, and a rough indication of the stiffness is given by the parameter  $E_{ii\_max}$ . For an isotropic material,  $E_{ii\_max}$  is the Youngs modulus *E*, while for an orthotropic material it is the maximum of  $E_{xx}$ ,  $E_{yy}$ , and  $E_{zz}$ . In addition, the total number of elements in the model having each material ID are shown, giving a measure of the distribution of the materials.

Table 2	2: Mate	erials			
Number of materials: 2					
m	ID	Name	Туре	E_ii_max	Elements
1	100	NewMaterial1	LinearIsotropic	6829.0	1351375
2	127	NewMaterial1	LinearIsotropic	6829.0	1316215

Note that in this example, it happens that although we have two material IDs (defined during segmentation), they are both assigned to the same material definition.

It is not feasible to list all parameters of the material definition in the analysis table, since the parameters required to characterize a material vary with the material type. If you require the exact material definitions, they can be obtained with the n88modelinfo command. For example

n88modelinfo --materials radius\_slice82\_bending.n88model

#### 6.3.2.3 Post-processing sets

The sets used by n88postfaim are reported. See Specifying post-processing node and element sets.

Table 3:	Post-processing	Sets		
Number o	f sets:			2
n	Node set name	Nodes	Element set name	Elements
1	face_z1	25991	face_z1	21210
2	face_z0	40032	face_z0	28999

### 6.3.2.4 Strain

Statistics of the six strain components for each element, namely the three engineering normal strains  $\varepsilon_{xx}$ ,  $\varepsilon_{yy}$ ,  $\varepsilon_{zz}$  and the three engineering shear strains  $\gamma_{yz}$ ,  $\gamma_{zx}$ ,  $\gamma_{xy}$ 

For models with elastoplastic material definitions, the strain given here is the total strain (*i.e.* the sum of the elastic and plastic strains).

The strains are summarized in terms of statistical quantities, namely average, standard deviation, minimum and maximum, and skewness and kurtosis. The median strain,  $5^{th}$ ,  $25^{th}$ ,  $75^{th}$  and  $95^{th}$  percentile strains are reported. Finally, the fraction of strains that are below zero (*i.e.* compressive strain) is reported in addition to the median and average strain of the negative (compressive) and positive (tensile) strain.

The summary of strains is provided for all elements in the model as well as being summarized for each specific material ID in the case of more than one defined material. In this example model, this provides a means of considering differences in the summary of strains in the cortex (*e.g.* material ID 127) separately from trabecular (*e.g.* material ID 100) bone.

Strain is dimensionless.

Table 4:	Strain					
m: Material	ID:					ALL ALL
average std_dev minimum maximum skewness kurtosis median perc05 perc25 perc75 perc95	epsilon_xx -3.190E-04 2.099E-03 -2.150E-02 1.734E-02 -7.522E-01 1.184E+00 -3.340E-05 -4.750E-03 -1.070E-03 7.472E-04 2.837E-03	epsilon_yy -1.595E-04 1.544E-03 -1.771E-02 2.012E-02 -1.510E-01 2.076E+00 -8.509E-06 -2.959E-03 -8.355E-04 5.336E-04 2.399E-03	epsilon_zz 5.405E-04 6.843E-03 -6.982E-02 7.162E-02 4.932E-01 3.916E-01 -1.603E-05 -9.953E-03 -3.705E-03 3.638E-03 1.409E-02	gamma_yz -7.457E-06 2.937E-03 -5.306E-02 4.388E-02 -8.113E-01 7.286E+00 1.328E-04 -5.143E-03 -9.735E-04 1.404E-03 4.025E-03	gamma_zx -2.048E-03 4.153E-03 -7.585E-02 4.232E-02 -9.770E-01 3.599E+00 -9.438E-04 -9.573E-03 -4.461E-03 3.828E-04 3.254E-03	gamma_xy -3.663E-05 1.403E-03 -3.298E-02 2.821E-02 6.881E-02 7.669E+00 -3.450E-05 -2.163E-03 -6.944E-04 6.016E-04 2.158E-03
m: Material  average std_dev minimum maximum	ID: epsilon_xx -3.326E-04 1.403E-03 -2.057E-02 1.734E-02	epsilon_yy -2.304E-04 1.296E-03 -1.771E-02 2.012E-02	epsilon_zz 9.468E-04 4.307E-03 -4.567E-02 6.647E-02	gamma_yz -2.711E-04 2.824E-03 -5.306E-02 4.388E-02	gamma_zx 8.815E-05 2.967E-03 -5.665E-02 4.232E-02	1 100 gamma_xy -1.733E-05 1.433E-03 -3.298E-02 2.821E-02

skewness	-9.487E-01	-5.547E-01	8.212E-01	-8.143E-01	-8.987E-01 -	-5.569E-02	
kurtosis	5.294E+00	4.647E+00	4.572E+00	1.121E+01	9.849E+00	1.051E+01	
median	-9.529E-05	-5.413E-05	1.652E-04	-1.758E-05	7.115E-05 -	-7.972E-06	
m:						2	
Material 3	ID:					127	
	•••••	•••••	•••••	•••••			
	epsilon_xx	epsilon_yy	epsilon_zz	gamma_yz	gamma_zx	gamma_xy	
average	-3.049E-04	-8.671E-05	1.232E-04	2.632E-04	-4.240E-03 -	-5.645E-05	
std_dev	2.629E-03	1.760E-03	8.690E-03	3.025E-03	4.054E-03	1.372E-03	
minimum	-2.150E-02	-1.667E-02	-6.982E-02	-3.880E-02	-7.585E-02 -	-1.501E-02	
maximum	1.322E-02	1.588E-02	7.162E-02	3.375E-02	2.053E-02	2.617E-02	
skewness	-6.398E-01	-3.604E-02	4.942E-01	-8.592E-01	-1.007E+00	2.105E-01	
kurtosis	-2.316E-01	7.413E-01	-7.675E-01	4.422E+00	3.701E+00	4.171E+00	
median	1 376E-04	9 347E-05	-2 057E-03	6 242E-04	-4 044E-03 -	-9 920E-05	

*Skewness* is a measure of the asymmetry of the distribution of element stresses. *Kurtosis* is a measure of the "peakedness" of the distribution of element stresses.

### 6.3.2.5 Plastic Strain

For models with elastoplastic material definitions, a table of plastic strain statistics is produced. To obtain the elastic strain, subtract the plastic strain from the total strain, given in the previous table.

The presentation of the plastic strain the same format as for the total strain.

Plastic strain is dimensionless.

Table 5:	Plastic Stra	Ln				
m: Material	ID:					ALL ALL
	•••••					•••••
	epsilon_xx	epsilon_yy	epsilon_zz	gamma_yz	gamma_zx	gamma_xy
average	-3.774E-04	-1.827E-04	5.602E-04	-2.491E-05	-1.051E-03	-4.255E-05
std_dev	2.441E-03	1.858E-03	4.103E-03	2.424E-03	3.285E-03	9.990E-04
minimum	-6.403E-02	-6.146E-02	-9.844E-02	-1.862E-01	-1.647E-01	-1.062E-01
maximum	4.919E-02	4.925E-02	1.223E-01	1.418E-01	1.750E-01	7.206E-02
skewness	-1.856E+00	-7.680E-01	1.454E+00	-3.772E+00	-3.946E+00	2.007E+00
kurtosis	1.172E+01	1.926E+01	1.147E+01	2.736E+02	8.944E+01	2.992E+02
median	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
perc05	-5.234E-03	-3.476E-03	-5.073E-03	-2.307E-03	-6.641E-03	-1.150E-03
perc25	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-9.717E-04	-5.828E-06
perc75	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
perc95	2.724E-03	2.380E-03	8.666E-03	2.226E-03	5.648E-04	9.484E-04
m:						1
Material	ID:					100
	ensilon xx	ensilon vv	ensilon 77	aamma vz		gamma xv
average	-2.516E-04	-2.011E-04	4.528E-04	-1.325E-04	-3.686E-05	2.363E-06
std dev	1.569E-03	1.441E-03	2.876E-03	2.513E-03	2.424E-03	9.711E-04
minimum	-6.084E-02	-6.146E-02	-9.844E-02	-1.862E-01	-1.647E-01	-1.062E-01
maximum	4.919E-02	4.925E-02	1.223E-01	1.418E-01	1.750E-01	6.961E-02
skewness	-4.158E+00	-3.443E+00	3.959E+00	-5.739E+00	-3.362E+00	5.373E-02
kurtosis	5.475E+01	5.797E+01	5.475E+01	4.191E+02	3.503E+02	4.686E+02
median	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
m:						2

Material ID:

```
127
```

	epsilon_xx	epsilon_yy	epsilon_zz	gamma_yz	gamma_zx	gamma_xy
average	-5.066E-04	-1.638E-04	6.704E-04	8.559E-05	-2.093E-03	-8.867E-05
std_dev	3.085E-03	2.205E-03	5.060E-03	2.324E-03	3.700E-03	1.025E-03
minimum	-6.403E-02	-4.663E-02	-7.185E-02	-1.076E-01	-1.294E-01	-2.535E-02
maximum	3.604E-02	4.230E-02	1.107E-01	8.670E-02	3.620E-02	7.206E-02
skewness	-1.209E+00	4.159E-02	7.811E-01	-1.199E+00	-4.140E+00	3.735E+00
kurtosis	4.603E+00	8.276E+00	3.481E+00	6.679E+01	4.224E+01	1.604E+02
median	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.584E-04	0.000E+00

## 6.3.2.6 Stress

Statistics of the six stress components for each element, including the normal stresses ( $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{zz}$ ) and shear stresses ( $\sigma_{yz}$ ,  $\sigma_{zx}$ ,  $\sigma_{xy}$ ).

The presentation of the stress follows the same format as described for the Strain table.

Units depend on inputs, but typically displacements are expressed in millimeters (mm), forces in newtons (N), and stresses in MPa. See Note about units.

Table 6:	Stress					
m:						ALL
Material	ID:					ALL
• • • • • • • • •					•••••	•••••
	SIGMA_XX	sigma_yy	SIGMA_22	sigma_yz	SIGMa_ZX	SIGMa_XY
average	-8.02/E-01	-5.936E-01	3.083E+00	-1.959E-02	-5.378E+00	-9.621E-02
sta_aev	1.315E+U1	1.070E+01	5.0/3E+01	1.204E+00	1.091E+01	3.686E+00
minimum	-Z.380E+02	-2.004E+02	-5.796E+U2	-1.394E+UZ	-1.992E+02	-8.662E+UI
maximum	1.682E+U2	1.632E+U2	5.51/E+UZ	1.153E+UZ	1.111E+U2	7.410E+01
skewness	-5.5/0E-01	4.960E-01	4.539E-01	-8.113E-01	-9.770E-01	6.881E-02
kurtosis	5.054E+00	4.068E+00	4.404E-01	7.286E+00	3.599E+00	7.669E+00
median	-4.492E-01	-3.217E-01	-2.718E-01	3.489E-01	-2.479E+00	-9.062E-02
perc05	-2.244E+01	-1.716E+01	-/.48/E+01	-1.351E+01	-2.514E+01	-5.681E+00
perc25	-7.064E+00	-5.724E+00	-2.868E+01	-2.557E+00	-1.172E+01	-1.824E+00
perc75	5.727E+00	2.874E+00	2.650E+01	3.687E+00	1.005E+00	1.580E+00
perc95	1.979E+01	1.944E+01	1.020E+02	1.057E+01	8.546E+00	5.668E+00
m:						1
Material	ID:					100
	•••••	•••••				
	sigma_xx	sigma_yy	sigma_zz	sigma_yz	sigma_zx	sigma_xy
average	6.726E-01	3.019E-01	6.486E+00	-7.120E-01	2.315E-01	-4.551E-02
std_dev	1.009E+01	7.009E+00	3.126E+01	7.418E+00	7.793E+00	3.764E+00
minimum	-1.424E+02	-1.625E+02	-3.346E+02	-1.394E+02	-1.488E+02	-8.662E+01
maximum	1.682E+02	1.632E+02	5.062E+02	1.153E+02	1.111E+02	7.410E+01
skewness	3.128E-03	4.413E-01	7.910E-01	-8.143E-01	-8.987E-01	-5.569E-02
kurtosis	8.270E+00	1.406E+01	4.799E+00	1.121E+01	9.849E+00	1.051E+01
median	8.653E-02	-4.944E-03	8.636E-01	-4.619E-02	1.869E-01	-2.094E-02
						2
Material	ID:					127
	sigma_xx	sigma_yy	sigma_zz	sigma_yz	sigma_zx	sigma_xy
average	-2.317E+00	-1.513E+00	-4.100E-01	6.914E-01	-1.114E+01	-1.483E-01
std_dev	1.554E+01	1.341E+01	6.472E+01	7.944E+00	1.065E+01	3.604E+00
minimum	-2.380E+02	-2.004E+02	-5.796E+02	-1.019E+02	-1.992E+02	-3.943E+01
maximum	1.506E+02	1.427E+02	5.517E+02	8.865E+01	5.392E+01	6.873E+01
skewness	-5.163E-01	5.951E-01	4.757E-01	-8.592E-01	-1.007E+00	2.105E-01
kurtosis	3 035E+00	1 604E+00	-7 415E-01	4 422E+00	3 701E+00	4 171E+00

median -3.882E+00 -2.612E+00 -1.698E+01 1.640E+00 -1.062E+01 -2.606E-01

### 6.3.2.7 Strain Energy Density

Statistics on the strain energy density are reported. See StrainEnergyDensity in Section 9.4 for a definition of the strain energy density.

For models with elastoplastic material definitions, the strain energy density is the elastic strain energy density. (Plastic strain energy density is not well defined: the work done producing a given a plastic strain is mostly converted into heat energy and cannot be retreived again as mechanical work.)

The presentation of the strain energy density follows the same format as described for the Strain table.

```
Table 7: Strain Energy Density
m:
                                                    ALL
Material ID:
                                                    ALL
......
average 2.091E-01
std_dev 3.039E-01
       5.704E-15
minimum
maximum
       2.186E+01
skewness 4.357E+00
kurtosis 9.588E+01
       8.209E-02
median
perc05
       4.649E-04
perc25
       1.149E-02
perc75
       2.918E-01
       8.012E-01
perc95
                                                     1
m:
Material ID:
                                                    100
average
        9.484E-02
std_dev
        2.108E-01
minimum
        5.704E-15
maximum
        1.662E+01
skewness
        7.458E+00
       1.533E+02
kurtosis
       1.993E-02
median
                                                     2
m:
                                                    127
Material ID:
average 3.264E-01
std_dev 3.382E-01
       1.353E-12
minimum
maximum
       2.186E+01
skewness 3.914E+00
kurtosis 9.946E+01
       2.203E-01
median
```

### 6.3.2.8 Von Mises Stress

Statistics on the von Mises stress are reported. See VonMisesStress in Section 9.4 for a definition of the von Mises stress.

The presentation of the von Mises stress follows the same format as for the Strain table.

Table 8: Von Mises Stress

111:		ALL
Material I	D:	ALI
average	3.920E+01	
std_dev	3.147E+01	
minimum	9.139E-06	
maximum	4.915E+02	
skewness	8.934E-01	
kurtosis	5.365E-01	
median	3.204E+01	
perc05	2.624E+00	
perc25	1.251E+01	
perc75	5.944E+01	
perc95	9.817E+01	
m:		
Material I	D:	100
average	2.455E+01	
std dev	2.461E+01	
minimum	9.139E-06	
maximum	4.237E+02	
skewness	1.832E+00	
kurtosis	4.876E+00	
median	1.643E+01	
m:		2
Material I	D:	127
average	5.423E+01	
std_dev	3.065E+01	
minimum	1.460E-04	
maximum	4.915E+02	
skewness	4.575E-01	
kurtosis	1.077E-01	
median	5.081E+01	

### 6.3.2.9 Nodal Displacements

The three components of displacements  $(u_x, u_y, u_z)$  are reported. A sub-table is generated for each post-processing node set. Statistics of the displacements are reported over all the nodes of each set.

Units are self-consistent, but are typically millimeters (mm). See A note about units.

Table 9: Nodal Displacements				
Node set: Name:				1 face_z1
average std_dev minimum maximum median	ux 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	uy 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	uz 8.493E-03 3.727E-02 -6.689E-02 7.695E-02 7.534E-03	
Node set: Name: average	ux 0.000E+00	uy 0.000E+00	uz 8.176E-03	2 face_z0

std_dev	0.000E+00	0.000E+00	5.033E-02
minimum	0.000E+00	0.000E+00	-8.768E-02
maximum	0.000E+00	0.000E+00	1.392E-01
median	0.000E+00	0.000E+00	1.250E-02

### 6.3.2.10 Nodal Forces

The three components of force  $(F_x, F_y, F_z)$  are reported. A sub-table is generated for each post-processing element set. The forces are provided giving statistical values over all elements in the set.

Units depend on inputs, but are typically Newtons (N). See A note about units.

```
Table 10: Nodal Forces
                 _____
Node set:
                                                         1
Name:
                                                    face z1
Fx Fy Fz
total -8.767E+02 -3.222E+00 5.025E+02
average -3.373E-02 -1.240E-04 1.933E-02
std_dev
        7.261E-02 3.936E-02 3.336E-01
minimum
        -8.420E-01 -3.484E-01 -2.614E+00
maximum 4.068E-01 6.302E-01 1.01
median -2.464E-02 -4.476E-04 4.233E-03
                                                         2
Node set:
Name:
                                                    face_z0
Fx Fy Fz
total
total 8.773E+02 3.162E+00 -5.032E+02
average 2.191E-02 7.898E-05 -1.257E-02
std_dev
       7.203E-02 5.302E-02 2.423E-01
minimum -3.655E-01 -3.909E-01 -1.399E+00
maximum 4.889E-01 3.679E-01 1.196E+00
median
        8.519E-04 -2.016E-03 3.913E-03
```

### 6.3.2.11 Nodal Twist

Similar to nodal displacements, statistics on the angular displacements for each node set are provided.

The angular displacements are defined as the projected angles between the vector to the initial location of the node and the vector to the displaced location of the node. The vectors are projected onto a plane perpendicular to the specified axis. This is shown in Figure 6.1, which defines ROTX. p is the initial position of the node, and p' is the displaced position of the node, as calculated by FE. These two vectors are projected onto the *y*-*z* plane, and the angle between them in this plane is defined as ROTX. ROTY and ROTz are similarly defined. Angular displacements are relative to the center of rotation; this is shown as  $p_0$  in the figure. See specifying a rotation center.



Figure 6.1: Definition of projected angle ROTx.

### Note

ROTx, ROTy, ROTz do not form a set of Euler angles.

Nodes that are within an exclusion radius (default value  $10^{-6}$ ) of the rotation center are excluded from the calculation, as the angular displacement of a node at the rotation center (initial or final position) is not defined.

## Units are radians (rad).

Table 11: Nodal Twist					
Twist measured relative to: Exclusion radius:				66.049 54.985 4.510 1.0E-06	
Node set: Name:				1 face_z1	
• • • • • • • • • •	ROTx	ROTy	ROTz		
n	25991	25991	25991		
average	5.978E-04	-3.252E-03	0.000E+00		
std_dev	3.424E-03	2.180E-03	0.000E+00		
minimum	-8.422E-03	-6.893E-03	0.000E+00		
maximum	7.567E-03	-6.411E-07	0.000E+00		
median	6.324E-04	-3.274E-03	0.000E+00		
Node set:				2	
Name:				face_z0	
	ROTx	ROTy	ROTz		
n	40032	40032	40032		
average	-7.531E-04	4.147E-03	0.000E+00		
std_dev	4.239E-03	2.363E-03	0.000E+00		
minimum	-1.014E-02	6.411E-07	0.000E+00		
maximum	9.126E-03	8.099E-03	0.000E+00		
median	-3.388E-04	4.688E-03	0.000E+00		

#### 6.3.2.12 Nodal Torques

Similar to nodal twist, statistics on the the nodal torques for each node set are reported.

As with the nodal twist results, torques are calculated relative to a reference point. See specifying a rotation center.

Units depend on inputs, but are typically in newton-millimeters (Nmm). See Note about units.

Table 12: Nodal Torques				
Torque measured relative to: 66.049 54.985 4.				
Node set: Name:				1 face_z1
total average std_dev minimum	Tx 1.094E+04 4.210E-01 2.312E+00 -5.420E+00	Ty -3.683E+04 -1.417E+00 1.847E+00 -2.341E+01	Tz -1.796E+03 -6.909E-02 7.455E-01 -9.929E+00	
maximum median	3.204E+01 2.183E-02	1.070E-01 -6.439E-01	5.532E+00 -2.549E-03	
Node set: Name:				2 face_z0
total average std_dev minimum maximum median	Tx -1.094E+04 -2.733E-01 1.487E+00 -1.111E+01 7.102E+00 -4.530E-03	Ty 3.682E+04 9.198E-01 1.466E+00 -3.944E+00 1.176E+01 3.083E-01	Tz 1.796E+03 4.486E-02 5.923E-01 -3.920E+00 5.743E+00 -2.374E-03	

### 6.3.2.13 Load Sharing

A calculation of the fraction of the load carried by each material ID is provided, based on the nodal forces in each associated node set.

The portion of total load on the node set is reported for each material in terms of nodal forces ( $F_x$ ,  $F_y$ ,  $F_z$ ). Nodal torques ( $T_x$ ,  $T_y$ ,  $T_z$ ) are also reported if a center of rotation is defined. See specifying a rotation center. The total forces and torques are also reported, and it should be noted that are the same as reported in Nodal Forces and Nodal Torques

The method used to determine the loads carried by each material requires identifying the nodes belonging to each material. Since material definitions are based on elements, some nodes are shared by more than one material. In these cases, the forces and torques associated with the node are proportionally assigned to each material definition.

```
Table 13: Load Sharing
_____
                  _____
Torque measured relative to:
                                   66.0487 54.9845 4.5100
       _____
                                _____
                                                 1
Node set:
Name:
                                             face z1
material Fx Fy Fz
              100 -2.2735E+02 2.2343E+01 1.5989E+02 ①
              127 -6.4936E+02 -2.5565E+01 3.4260E+02
          _____
                  _____
                          _____
                                  _____
             total -8.7671E+02 -3.2224E+00 5.0249E+02 2
                       Tx
           material
                               Ту
                                       Τz
              100 1.3237E+03 -4.6310E+03 -5.3746E+02
               127 9.6174E+03 -3.2197E+04 -1.2583E+03
                  _____
                          _____
             total 1.0941E+04 -3.6828E+04 -1.7958E+03
```

Node set: Name:					2 face_z0
	material 100 127 	Fx -8.0150E+01 9.5741E+02  8.7726E+02	Fy 1.3524E+02 -1.3208E+02  3.1616E+00	Fz -2.2235E+02 -2.8086E+02  -5.0321E+02	
	material 100 127 	Tx -4.4656E+03 -6.4737E+03  -1.0939E+04	Ty 1.5580E+04 2.1242E+04  3.6823E+04	Tz 1.3600E+02 1.6599E+03  1.7959E+03	

- Represents the total force attributed to material definition 127 (cortical bone in this model).
- 2 This result is the same as the total  $F_z$  in Nodal Forces.

# 6.4 Tabulating results from analysis files

The analysis file generated by n88postfaim is intended to be human-readable. If you run several similar models, it is common to want to tabulate certain numerical results in spreadsheet format. It is possible, but tiresome, to open the analysis file for each solved model individually and manually search for the desired numbers. To make this process more efficient, we provide the tool n88tabulate. See Section 9.14. This tool extracts certain specified values from any number of analysis files and collates them into a tabular format suitable for importing into a spreadsheet.

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# **Chapter 7**

# **Tutorials**

This chapter presents a number of tutorials to help you learn the Faim finite element tools.

The first series of tutorials introduces the standard work flow for Faim, where standard models as generated by n88modelgenerator are desired. These tutorials are

- 1. An introductory tutorial: compressing a solid cube
- 2. Compression test of a radius bone slice
- 3. Bending test of a radius bone with an uneven surface

These are intended to be followed in order, as each one builds on the previous.

Following these introductory tutorials is a series dealing with more advanced topics

There is a tutorial that introduces models with nonlinear elasto-plastic material properties.

1. Bending of a radius bone with elasto-plastic material properties.

Then there are a series of tutorials which present the building of custom models using vtkn88. This series is intended only for those who find n88modelgenerator insufficiently flexible for their needs. The tutorials in this series are

- 1. Compressing a cube revisited using vtkn88
- 2. Deflection of a cantilevered beam; adding custom boundary conditions and loads
- 3. A cantilevered beam with elastoplastic material properties
- 4. Advanced custom model tutorial: a screw pull-out test

Finally, some additional examples are provided with the distribution. These are not described in the manual, but do demonstrate addition concepts or functionality.

# 7.1 Introductory tutorial: Compressing a solid cube

We start with a very simple example, where we compress a uniform homogenous cube. This tutorial will demonstrate:

- How to use the standard test generator n88modelgenerator to generate a finite element model suitable for input to the solver.
- How to solve the model.

- How to use ParaView to visualize the model and the solution.
- How to identify key values in the analysis file.

The data file is cube6x6x6.vti. It can be found in the data folder of the distribution. We recommend that you copy it to a temporary working directory for this tutorial.

You can examine this data file, which we will be using as input, with ParaView. To do this, open ParaView and select the menu item File  $\rightarrow$  Open, and navigate to the location of cube6x6x6.vti. You will notice that after selecting the file and clicking OK, nothing is displayed, although the file name now appears in the "Pipeline Browser". This is typical for ParaView, and allows options relevant to the source to be modified before the data is actually loaded. In this case, there are no options we are concerned with, so we can go ahead and click the Apply button (on the Properties tab of the Pipeline browser) to actually load the data. At first, only a wire-frame cube will be displayed, which shows the extents of the image data. To actually inspect the data, we are going to change the drop-down list on the toolbar that currently displays "Outline" to "Points". This results in a display of a number of points in space, as shown in Figure 7.1.



Figure 7.1: Points view of 6x6x6 cube.

If you're alert, you'll notice that in fact there are  $7 \times 7 \times 7$  points. This is due to the fact that the actual data for this data file is associated with the "Cells", to use VTK terminology, rather than the "Points". The points shown are therefore in this case the corners of the cells. To make this clear, change the view again from "Points" to "Surface with Edges". This will now look like Figure 7.2. (Click and drag in the image window of ParaView to rotate the object - experiment with both the right and left mouse buttons, and also while holding down any of the Shift, Control and Alt keys). We are going to create a finite element model where every "Cell", or small constituent cube from Figure 7.2 will become one element in the finite element model.



Figure 7.2: Surface with edges view of 6x6x6 cube.

For a simulated test, we are going to apply a compression test using n88modelgenerator to this data file. There are a number of different standard compression tests, as described in Standard Tests. Here we are going to use the axial variation. In an axial compression test, the sides are unconstrained and the top and bottom surfaces constrained laterally, as if they experience a high contact friction with the imaginary surfaces applying the compression.

## 7.1.1 Generating the model

The first step is to open a terminal (called a Command Prompt on Windows and Terminal on OS X) and make sure the environment variables are set as described in Setting environment variables.



### Important

If you close the command prompt window part way through this tutorial, and then pick it up again later by opening a new command prompt window, you will have to re-set the environment variables as described in Setting environment variables.

Assuming that you have copied the data file cube6x6x6.vti, the command to generate the model is

```
n88modelgenerator --test=axial cube6x6x6.vti
```

If you haven't copied the file cube6x6x6.vti to your working directory, then you will need to specify the complete path, for example as "/Applications/Faim 7.1/data/cube6x6x6.vti" on OS X.

Since we haven't specified otherwise, n88modelgenerator will select all default parameters, including default material properties (homogeneous material with isotropic Young's modulus of 6829 MPa), and a displacement, applied to the top surface in the *z* direction, numerically equivalent to an apparent level strain of -0.01 (the minus indicates compressive strain). Refer to the section on n88modelgenerator for details on setting parameters differently if you wish to do so.

Here is the output when we run it:

```
Copyright (c) 2010-2015, Numerics88 Solutions Ltd.
Licensed to Numerics88 Solutions Ltd.; lic. no. 91
input_file = cube6x6x6.vti
output_file = cube6x6x6_axial.n88model
                              = axial
test
                              = z
test axis
normal strain
                              = -0.01
                             = intersection
top_surface
bottom_surface
                             = intersection
material_table
                             = homogeneous
youngs_modulus
                             = 6829
poissons_ratio
                             = 0.3
connectivity_filter
                              = on
  0.02 Reading input data.
   0.04 Read 343 points.
   0.04 Image bounds:
       0.0000 6.0000 0.0000 6.0000 0.0000 6.0000
   0.04 Applying connectivity filter.
   0.04 Masked out 0 unconnected voxels.
   0.04 Converting to hexahedral cells.
   0.04 Generated 216 hexahedrons.
   0.04 Constructing material table.
   0.05 Material table has 1 entry.
   0.05 Constructing finite element model.
   0.05 Model bounds:
        0.0000 6.0000 0.0000 6.0000 0.0000 6.0000
   0.06 Generated the following constraints:
          bottom_fixed : 147 nodes
          top_fixed : 98 nodes
          top_displacement : 49 nodes
   0.06 Writing Numerics88 Model file cube6x6x6_axial.n88model .
   0.09 Done.
```

We now have a file cube6x6x6\_axial.n88model that can be used directly as input to the solver.

# 7.1.2 Solving the model

Having now defined the problem, we can solve it, and do some post-processing, all in one step with faim.

```
faim cube6x6x6_axial.n88model
```

### The output is:

```
Model contains only linear material definitions.
Choosing solver_sl.
Running solver: n88solver_sl cube6x6x6_axial.n88model
n88solver_sl version 7.1
Copyright (c) 2010-2015, Numerics88 Solutions Ltd.
Licensed to Numerics88 Solutions Ltd.; lic. no. 91
Problem:
    active solution : (none)
    active problem : Problem1
    number of elements : 216
    number of nodes : 343
Engine: mt
Precision: double
Using 1 engine thread(s).
```

```
Solver parameters:
 convergence tolerance = 1e-006
 threshold window
                   = 3
 maximum iterations = 30000
              iter
   time (s)
                             conv
        0.0
                28
                        8.6E-08
Linear iterations: convergence measure tolerance reached.
Number of linear iterations = 28
Peak data allocation : 93.4 kiB
Running field calculator: n88derivedfields cube6x6x6_axial.n88model
n88derivedfields version 7.1
Copyright (c) 2010-2015, Numerics88 Solutions Ltd.
Licensed to Numerics88 Solutions Ltd.; lic. no. 91
Problem:
 active solution
                     : Solution1
                  : Problem1
 active problem
 number of elements : 216
 number of nodes
                   : 343
Precision: single
Peak data allocation: 22.1 kiB
Running analysis tool: n88postfaim --output_file cube6x6x6_axial_analysis.txt ↔
   cube6x6x6_axial.n88model
```

## 7.1.3 Visualizing the results with ParaView

First ensure that ParaView is set up with the plugins to read Numerics88 files, as described in Installing and using the Numerics88 plugins for ParaView. Assuming that the plugins are loaded correctly, cube6x6x6\_axial.n88model can be opened directly with ParaView. When we first open this file, it looks very similar to the input data. However, if we go to the "Information" tab in the Pipeline Browser, we can see that there are now several Data Arrays, "Displacement", "ReactionForce", etc... as shown in Figure 7.3. Notice that the icon next the the array name indicates whether the data is on "Points" or "Cells", which is equivalent in finite element terminology to "Nodes" and "Elements", respectively.



Figure 7.3: Solved 6x6x6 cube with Data Arrays.

There are many ways to visualize the data. As a simple example, choose "Displacement" from the drop-down menu on the toolbar that currently shows "MaterialID". Also click the "Toggle Color Legend Visibility" button on the toolbar (on the very left side). ParaView should now look like Figure 7.4. Notice that a new drop-down box appears that shows "Magnitude". This occurs because the Displacements are a vector quantity. Experiment with changing this to "Z", "X" and "Y".



Figure 7.4: Solved 6x6x6 cube colored by Displacement.

Although we now have the cube colored by Displacement, the object is shown in its undeformed unloaded shape. To visualize the deformations, we can use the "Warp By Vector" tool. There is an icon for this on the bottom Toolbar. Because we have imposed a small strain, -0.01, it will be hard to see. The "Warp By Vector" tool however allows us to apply a Scale Factor. We will set this to 10, so that the displacements are amplified by a factor of 10. The results are shown in Figure 7.5, where the compression and outward bulging of the sides are clearly seen. In this figure, we have, in addition to applying the Warp By Vector tool, re-enabled the display of the original cube $6x6x6\_axial.n88model$ , which was automatically disabled by ParaView when we connected a filter object to it. We then set its display type to "Outline", resulting in the white box outline in Figure 7.5, which indicates the original undeformed box shape.



Figure 7.5: Solved 6x6x6 cube shown with exaggerated displacement using the Warp By Vector tool.

## 7.1.4 Obtaining numerical values from the analysis file

A typical result we want to obtain with a compression test is the object apparent stiffness. Numerically the stiffness is the net external force divided by the displacement. We can find the displacement and force on the top surface from the analysis file, cube6x6x6\_axial\_analysis.txt. This file is a text file, and can be opened with any text editor. Refer to the section on post-processing with n88postfaim for the complete explanation of the values available.

The displacement is obtained from table Nodal Displacements. The displacements in this table are listed according to node set.

n88modelgenerator has defined some standard node sets (for a complete list see Creating node and element sets in the chapter on Preparing Models with vtkn88.) Here the node sets that are relevant are the two surfaces to which the boundary conditions are applied, namely the top and bottom surfaces, "face\_z1" and "face\_z0", respectively. The analysis file has been generated using these two node sets. If we examine the Nodal Displacements table of cube6x6x6x\_axial\_analysis.txt, as shown in Figure 7.6, we see that the top node set has a uniform displacement in the z direction of -0.06 mm. The relevant number is circled in red. Notice also that the minimum and maximum are the same so all nodes of this set are equally displaced, as we expect, since this is in fact a boundary condition. The other node set is the nodes of the bottom surface, and it has constant displacement of 0.

	odal Displac	ements		 
Node set: Name:				 1 face_z1
average std_dev minimum maximum median	UX 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	Uy 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	-6.000E-02 0.000E+00 -6.000E-02 -6.000E-02 -6.000E-02	
Node set: Name:				 2 2 face_z0
average std_dev minimum maximum median	U.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	uy 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	UZ 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	

Figure 7.6: uz components in Nodal Displacements table of the analysis file.

1		
face_z1		Name:
•••••	Fx Fy Fz	•••••
	-7.629E-06 -1.144E-05 -2.652E+03	total
	-1.557E-07 -2.336E-07 -5.411E+01	average
	1.025E+01 1.025E+01 1.251E+01	std_dev
	-1.898E+01 -1.898E+01 -6.776E+01	ninimum
	1.898E+01 1.898E+01 -2.834E+01	nax1mum modion
2		Node set:
1ace_20		vane:
	Fx Fy Ez	
	4.292E-06 -2.384E-06 2.652E+03	total
	8./58E-08 -4.866E-08 5.411E+01	average
	1.025E+01 1.025E+01 1.25IE+01 _1.008E+01 _1.008E+01 2.034E+01	sta_aev
	1 898E+01 1 898E+01 6 776E+01	maximum
	0 000E+00 0 000E+00 6 406E+01	median

Figure 7.7: Fz components in Nodal Forces table of the analysis file.

Similarly to the table for displacements, table Nodal Forces shows forces, summed over the defined node sets. Here the relevant value is -2651 N, as shown in Figure 7.7. The apparent stiffness of the cube is therefore

$$\frac{-2651N}{-0.06\,mm} = 4.42 \times 10^5 N/mm$$

Is this value reasonable? We can estimate what we should get. Completely ignoring lateral expansion and Poisson's ratio, we

can do a quick estimate that the stiffness of a homogeneous cube should be approximately,

$$k = \frac{Eh}{A} = \frac{(6829 N/mm^2)(6 mm)^2}{(6mm)} = 4.10 \times 10^5 N/mm$$

This is close to what we obtained from the finite element model. The difference arises from the fact that the finite element model takes account of the complicated lateral expansion (bulging of the sides) that occurs in an axial test, while our simple back-of-the-envelope calculation assumes uniaxial conditions (*i.e.*, no lateral constraint on the top and bottom boundary surfaces).

This concludes the cube tutorial. You have learned how to generate standard models from image data using n88modelgener ator, how to solve the models, how to visualize the models using ParaView, and how to do some elementary post-processing analysis.

# 7.2 Tutorial: Compression test of a radius bone slice

In the previous tutorial, we saw how to generate a finite element model from an image file using n88modelgenerator, how to solve it, how to visualize the results, and how obtain some relevant numerical results. In this tutorial, we are going to generate and solve a similar compression test. Instead of a small contrived image, we will be using a real data file obtained from a microCT scan of a distal radius bone. We will also provide more detail about the steps along the way, and be introduced to some of the tools that aid in examining and verifying models.

In detail, this tutorial will demonstrate:

- How to use n88modelinfo to obtain information about n88model files, and in particular to trace back exactly how they were generated and processed.
- How to examine the residuals to evaluate the accuracy of the solution.
- How to quantify the load sharing between the two types of bone, cortical bone and trabecular bone.
- How to compress data files using n88copymodel for efficient storage.

The data file is radius\_slice82.aim, and it can be found in the data directory of the distribution. This is a large image file of  $325 \times 437 \times 110$  voxels in size. It was obtained with a scan resolution of 82 micrometers. The tutorial will be demonstrated using this data file. However, a reduced-resolution file, radius\_slice164.aim, is also provided. The resolution has been reduced to an effective 164 micrometers, resulting in a much smaller data file with dimensions  $163 \times 219 \times 55$ . If you are working on a computer with limited memory, or are just impatient, then you can follow along using the smaller file.

Before proceeding, ensure that the Numerics88 plugins are loaded as described in Installing and using the Numerics88 plugins for ParaView.

In the previous tutorial you might recall that the data file was a VTK image data file, and that it explicitly had the data on the "Cells" rather than on the "Points". Most image file formats make no such distinction, but ParaView always uses one or the other, as it affects how the data are rendered. In fact if you experiment you will determine that certain filters will work in one case and not the other, or that other filters will work differently depending on whether the data are on the Points or the Cells. As an example, the "Contour" filter requires data on the Points, while the "Threshold" filter generally only gives the results you expect with the data on the Cells. You will see when opening an AIM file that in the Properties tab we have a couple of options, which are "Data on Cells" and "Pad". This is shown in Figure 7.8. For this tutorial we want to select "Data on Cells", which is the default.



00	M ParaView 3.14.1 64-bit	
1 10 10 10 10 10 10 10 10 10 10 10 10 10	? 🔍 🗛 🗛 🕸 🔅	🕺 🕅 🗐 🕨 🕪 🕅 🛱 Time: 💽
:	Representation      *	5 🗱 🗱 👯 🗱 😫 🖉 🖉 »
	õ 🙆 😒	
Pipeline Browser	00	Layout #1 🙁 +
builtin: radius_slice82.aim  Properties Display Information Properties  Apply @ Reset & Delete  Data on Cells Pad		
	k γ	
	*	

Figure 7.8: Options when opening an AIM file.

Once you've opened the file radius\_slice82.aim (or radius\_slice164.aim) and clicked Apply, locate the icon for the Threshold filter on the toolbar. Change the Lower Threshold to 1 before clicking Apply, as shown in Figure 7.9; Scalars should be set to "AIMData".

000	/// ParaView 3.14.1 64-bit
6 6 😨 🦉 🔊 🖉 😭	🗼 📉 🔯 🕸 🕸 🔣 🐁 🖂 🗐 🕨 🕪 🔛 😫 Time: 💽 <sup>34</sup>
Solid Color +	Representation : 🔀 😳 🗱 😫 🕌 🗳 🗸 🖧 💋 »
🗐 💊 🕫 🕸 🧐 🔮 🥖	6 6 1
Pipeline Browser 💿 😒	Layout #1 😒 +
<ul> <li>builtin:</li> <li>radius_slice82.aim</li> <li>Threshold1</li> <li>Properties</li> <li>Display</li> <li>Information</li> <li>Properties</li> <li>Scalars</li> <li>AIMData</li> <li>Lower Threshold</li> <li>1</li> <li>Upper Threshold</li> <li>127</li> <li>All Scalars</li> </ul>	

Figure 7.9: The threshold filter.
Now change the "Representation" drop-down box to "Surface" and the "Color by" drop-down box to "AIMData". Also turn on the legend by clicking the "Toggle Color Legend Visibility" button. After rotating the image (click and drag in the image window) to get a good viewing angle, this should look something like Figure 7.10. You can see that this data file has been segmented such that the cortical bone has material ID 127 and the trabecular bone has material ID 100.



Figure 7.10: Input image for the radius slice tutorial.

# 7.2.1 Generating the model

As before, we recommend copying the data file radius\_slice82.aim into a temporary working directory. The command to generate the model is

n88modelgenerator --test=uniaxial radius\_slice82.aim

The resulting model file will be named radius\_slice82\_uniaxial.n88model.

#### Note

Don't forget that before running n88modelgenerator, you'll need to set environment variables as described in Setting environment variables.

Now before we solve it, we are going to examine this model file using n88modelinfo. You will find that n88modelinfo is a very useful tool for getting information about the models, and for tracing back how they were created and solved. n88modelinfo can be run like this,

n88modelinfo radius\_slice82\_uniaxial.n88model

n88modelinfo can generate quite a bit of output. We will shortly see how to reduce this to just the information that we are interested in. For now though, let's look at the complete output. Comments follow below the example output.

History:

2015-Sep-20 16:29:03 Model created by n88modelgenerator version 7.1 Log: \_\_\_\_\_ 2015-Sep-20 16:29:03 n88modelgenerator Licensed to Numerics88 Solutions Ltd.; lic. no. 91 input\_file = radius\_slice82.aim output\_file = radius\_slice82\_uniaxial.n88model test = uniaxial test\_axis = z normal\_strain = -0.01pin = off top\_surface = intersection = intersection bottom\_surface = homogeneous material\_table = 6829 youngs\_modulus = 0.3 poissons\_ratio connectivity\_filter = on \_\_\_\_\_ Active Settings: \_\_\_\_\_ Active Solution : None Active Problem : Problem1 Active Part : Part1 Materials: Name : NewMaterial1 Type : LinearIsotropic E : 6829.0 nu : 0.3 \_\_\_\_ \_\_\_\_\_ Parts: \_\_\_\_\_ Name : Part1 NumberOfNodes : 3816642 Hexahedrons : NumberOfNodesPerElement : 8 NumberOfElements : 2667590 \_\_\_\_\_ \_\_\_\_\_ Constraints: \_\_\_\_\_ Name : bottom\_fixed Part : Part1 Type : NodeAxisDisplacement NumberOfValues : 40032 Name : top\_displacement Part : Part1 Type : NodeAxisDisplacement NumberOfValues : 25991

\_\_\_\_\_

NodeSets: \_\_\_\_\_ \_\_\_\_\_ Name : face\_z0 Part : Part1 NumberOfNodes : 40032 Name : face\_z1 Part : Part1 NumberOfNodes : 25991 Name : face\_x0 Part : Part1 NumberOfNodes : 15 Name : face\_x1 Part : Part1 NumberOfNodes : 14 Name : face\_y0 Part : Part1 NumberOfNodes : 27 Name : face\_y1 Part : Part1 NumberOfNodes : 17 \_\_\_\_\_ \_\_\_\_\_ \_\_\_\_ ElementSets: Name : face\_z0 Part : Part1 NumberOfElements : 28999 Name : face\_z1 Part : Part1 NumberOfElements : 21210 Name : face\_x0 Part : Part1 NumberOfElements : 8 Name : face\_x1 Part : Part1 NumberOfElements : 6 Name : face\_y0 Part : Part1 NumberOfElements : 12 Name : face\_y1 Part : Part1 NumberOfElements : 8 \_\_\_\_\_ \_\_\_\_\_ Problems: \_\_\_\_\_ \_\_\_\_

Name : Problem1

Some things to note about the output of n88modelinfo:

- The "History" is a useful field to see what programs were run to generate or modify the file, and when.
- The "Log" field is similar to the History, except that it gives far more detailed information. Of particular note is that n88modelgenerator reports its complete configuration, including all parameters values relevant to the particular test type, even ones which haven't been explicitly set, but are default values.
- This file hasn't been solved yet, so there is nothing in "Solutions".
- The sets defined for post-processing are "face\_z1" and "face\_z0", which are the top and bottom surfaces, respectively. We will need this information later to interpret the results in the analysis file.

Now, as mentioned, that is a lot of output. Often we are interested in just part of the output. In this case, we can specify the bits we want. For example, to get just the History and the Log, we could do this,

n88modelinfo --history --log radius\_slice82\_uniaxial.n88model

Tip

To discover what the valid arguments to n88modelinfo are, you can either refer to the manual (See Section 9.10), or you can run n88modelinfo --help.

#### Tip

If you want the output of n88modelinfo to be saved in a file, then run it like this

n88modelinfo radius\_slice82\_uniaxial.n88model > info.txt

This will direct the output of n88modelinfo to the file info.txt.

# 7.2.2 Solving the model

From the previous tutorial, we know that we can use faim to solve the model and perform so post-processing on it. faim itself actually just calls three other programs to carry out the actual work. Usually it's easiest to call faim, but in this tutorial we are going to call the individual processing programs ourselves, so we can understand what faim is doing.

The first step carried out by faim is to solve the model with n88solver\_sl, which we can do with

```
n88solver_sl radius_slice82_uniaxial.n88model 0
```

• The specification sl for the solver means that this is the solver for *small strain* and *linear* problems.

#### Tip

This model will take some time to solve. If you have licensed the GPU solvers, and have suitable hardware, then you probably would like to jump right into using the GPU hardware. To do this, specify the engine and device. For example, for a system with two compute-capable NVidia cards, including the one being used for the display, the command would be:

n88solver\_sl --engine=nv --device=0,1 radius\_slice82\_uniaxial.n88model

If you have a system where the compute GPUs are distinct from the video card used for the display, such as is typical for nVidia Tesla hardware, then the correct device option for two compute-capable NVidia cards is more likely to be --device=1, 2.

We can see how this has modified the n88model file by running n88modelinfo again. To avoid the lengthy complete output, here we use arguments that show only the sections that have in fact changed

n88modelinfo --history --log --solutions radius\_slice82\_uniaxial.n88model

#### The output is:

#### History:

2015-Sep-20 16:29:03 Model created by n88modelgenerator version 7.1 2015-Sep-20 16:33:39 Solved by n88solver\_sl 7.1

Log:

```
2015-Sep-20 16:29:03
n88modelgenerator
Licensed to Numerics88 Solutions Ltd.; lic. no. 91
input_file = radius_slice82.aim
output_file = radius_slice82_uniaxial.n88model
test
                              = uniaxial
test_axis
                              = z
normal_strain
                              = -0.01
                              = off
pin
top_surface
                              = intersection
bottom surface
                              = intersection
material_table
                              = homogeneous
youngs_modulus
                              = 6829
poissons_ratio
                              = 0.3
connectivity_filter
                              = on
2015-Sep-20 16:33:39
n88solver_sl version 7.1
Copyright (c) 2010-2015, Numerics88 Solutions Ltd.
Licensed to Numerics88 Solutions Ltd.; lic. no. 91
Problem:
 active solution : (none)
active problem : Problem1
 number of elements : 2667590
 number of nodes
                     : 3816642
Engine: nv
Precision: double
Using 2 engine thread(s).
Solver parameters:
 convergence tolerance = 1e-006
 threshold window = 3
 maximum iterations = 30000
Linear iterations: convergence measure tolerance reached.
Number of linear iterations = 4848
Peak data allocation of supervisory thread: 408 MiB
```

```
Peak data allocation, sum over worker threads (system, device): 2.32 GiB, 0
------
Solutions:
------
Name : Solution1
Problem : Problem1
Variables defined on nodes:
   Displacement
```

Note things are worth noting here. In the Log section, we now have a record of the complete configuration of the solver (in this case, it happens to be default values). And in the Solutions section, we now have a solution ("Solution1") with a field defined on the nodes, namely "Displacements".

### 7.2.3 Evaluating the accuracy of the solution

Faim includes a tool that can be used to evaluate the accuracy of the obtained solutions. This is discussed in the section Evaluating solution quality. It can be run like this:

n88evaluate radius\_slice82\_uniaxial.n88model



Warning

The n88evaluate tool in its current implementation requires far more memory than the solver itself does. For this example, it will use almost 60GB of memory, while the solver needed less than 2GB. Therefore, currently, you should not attempt to run this part of the tutorial on a machine with less than 64GB of RAM.

The output is,

```
Analysis of solution displacements at boundary conditions:
  max err : 0.00E+00
  rms err : 0.00E+00
Analysis of forces (residuals):
  max err : 1.28E-05
  rms err : 9.35E-07
  max err/max force : 9.26E-06
  rms err/max force : 6.79E-07
```

The meaning of these results is discussed the section Evaluating solution quality; briefly we can take the number rms err/max force as a measure of the relative error. Here it is  $7 \times 10^{-7}$ , which is acceptably small.

# 7.2.4 Obtaining additional solution fields with n88derivedfields

So far our solution consists only of displacements. Many other values are of interest, for example strains and stresses. These are calculated with n88derivedfields. It can be run very simply as,

n88derivedfields radius\_slice82\_uniaxial.n88model

Now let's have a look at what's in the model file, using again n88modelinfo,

n88modelinfo --history --solutions radius\_slice82\_uniaxial.n88model

The output is:

```
History:

2015-Sep-20 16:29:03 Model created by n88modelgenerator version 7.1

2015-Sep-20 16:33:39 Solved by n88solver_sl 7.1

2015-Sep-20 16:41:12 Processed by n88derivedfields 7.1

Solutions:

Name : Solution1

Problem : Problem1

Variables defined on nodes:

Displacement

ReactionForce

Variables defined on elements:

Strain

Stress

StrainEnergyDensity

VonMisesStress
```

We have a number of new solution fields (or variables). Some are defined on the nodes and some defined on the elements. For details on these fields, see Section 9.4.



#### Important

Even if you are not interested in the numerical values of the fields added by n88derivedfields, they are required by n88postfaim. Running the latter requires first running the former.

### 7.2.5 Using n88postfaim to generate the analysis file

The final step performed by faim is to call n88postfaim, which does post-processing analysis. In the previous tutorial we saw that an analysis file was generated, which is a text file with a number of tables summarizing the numerical results. It is n88postfaim that generates this text file. To run it on an n88model file that contains all the solution fields is once again straightforward in most cases,

n88postfaim -o analysis.txt radius\_slice82\_uniaxial.n88model

Note that unlike the previous commands, for n88postfaim we actually have to specify an output file with -o analysis. txt. (If we don't, then the output will just be printed to the terminal.) The faim command, which combines n88solver, n88derivedfields, and n88postfaim, would have automatically generated the filename radius\_slice82\_uniaxial\_ana lysis.txt in this case, but that is getting a little bit lengthy, so we'll just use analysis.txt here.

### 7.2.6 Determining load sharing distribution with n88postfaim

We already saw some of the values in the analysis file in the previous tutorial. For this tutorial, we are going to have a look at table Load Sharing, as shown in Figure 7.11. We see that this table breaks up the total load on each node set according to material ID. In this case, we have material ID 127 being cortical bone, and material ID 100 being trabecular bone. Recall that the material properties are not different; it is merely a different labelling. Here we will see the reason for doing this. Recall also that the sets defined for post-processing are the top and the bottom surfaces. (If you're not sure of this then the command n88modelinfo --problems radius\_slice82\_uniaxial.n88model will show you.) Because of the alignment in the CT scanner, in this case the top surface is proximal, and the bottom surface is distal. Referring to the values circled in red in Figure 7.11, we conclude that on the proximal surface of this radius bone slice, the proportion of the load carried by the trabecular bone is (-806)

Node set: Name:					1 face_z1
	material 100 127	Fx 1.0137E-04 -3.2226E-05	Fy -2.2674E-03 -3.6492E-03	Ez -8.0637E+02 -4.3925E+03	
	total	6.9141E-05	-5.9166E-03	-5.1989E+03	
Node set: Name:					2 face_z0
	material 100 127	Fx -4.4259E-04 -2.3249E-04	Fy 1.4618E-04 7.4923E-05	Fz 3.6373E+03 1.5674E+03	
	total	-6.7508E-04	2.2110E-04	5.2046E+03	

Figure 7.11: Load Sharing table in analysis file.

# 7.2.7 Enabling compression for large model files

The n88model file format supports compression internally and transparently. An n88model which contains compressed data can be read with every N88 tool just like any other n88model, without the need for the user to explicitly de-compress the data. Compression is not used by default, because it does have an increased calculation overhead for reading and writing (particularly for writing). However, once we are finished with processing the model, we typically want to keep the data around for archival purposes. It is recommended to compress the n88model files for archiving. This can be done with the n88compress tool, as follows,

n88compress radius\_slice82\_uniaxial.n88model

For this data file, enabling compression reduces its size from 394 MB to 219 MB, a reduction of 44%.

This ends the tutorial on a compression test on a radius bone slice. We were introduced to n88modelinfo, we solved a realistic model, we looked at using the residuals to evaluate the quality of the solution, we saw how to do load distribution calculations, and finally we learned how to enable compression to more efficiently store large n88model files.

# 7.3 Tutorial: Bending test of a radius bone with an uneven surface

In the previous two tutorials, we had input images where the object in the image intersected the top and bottom bounds of the image, thus forming nice flat surfaces to which we could apply boundary conditions. This won't always be the case. In this tutorial we'll look at an object with a very uneven surface.

In detail, this tutorial will demonstrate:

- How to use the uneven surface parameters of n88modelgenerator.
- How to use n88extractsets to examine our boundary conditions.

The data file is radius82.aim. As for the previous tutorial, there is also a reduced resolution version, radius164.aim. This data is particularly large, with the unreduced version having a size of  $400 \times 350 \times 1100$ , or 154 million voxels; the resulting finite element model will have 14 million elements.

The input image is shown in Figure 7.12.



Figure 7.12: Radius bone image for bending test.

### Тір

In this tutorial, we are no longer going to go into detail on how to load and render data in ParaView, as we did in the previous two tutorials. If you're curious about how we generated that image of the radius bone from the image file, these are the steps:

- 1. Open the  ${\tt radius82.aim},$  and before clicking Apply, deselect Data on Cells
- 2. Add a Contour filter. The default contour value (63.5) is fine.
- 3. In View Options, add a Headlight with value 0.06.

# 7.3.1 Generating the model with n88modelgenerator

We are going to apply a bending test, as described in Bending test. In order to identify the rough head of the bone as a boundary surface, we use the option bottom\_surface=visible. As it implies, it will select nodes that are visible from a certain point of view.

In this case, visible means "looking up from below" (effectively from an infinite distance, as parallel rays are used). Note that the distal head of the bone is in the "bottom" of the image, that is at smaller values of *z*. With this option, you can imagine that we might "see" parts of the object that are far away if they are not obscured by the foreground part of the image. We don't want these distant parts of the object to form part of our boundary set, so when we use the bottom\_surface=visible option, we nearly always want to set a depth limit as well using bottom\_surface\_maximum\_depth. In this case a suitable limit is 15 (units are the same as the image units, which are millimeters in this case). In general there may be a bit of experimentation to get the best depth limit.

Since we have several parameters that we want to specify, it will be more convenient to create a configuration file for n88modelgenerator than to specify them individually on the command line, as we have done previously. To do this, open a text editor, and create the following file. Save it to your working directory as radius\_bending\_test.conf.

```
# File: radius_bending_test.conf
#
# A configuration file for the radius bending tutorial.
input_file = radius82.aim
test = bending
bottom_surface = visible
bottom_surface_maximum_depth = 15
```

Lines starting with # are comment lines: any line starting with # is ignored.

We can now run n88modelgenerator by specifying only the configuration file to use:

n88modelgenerator --config radius\_bending\_test.conf

Tip

Some text editors automatically add a .txt file extension. You can either subsequently rename the file, or just accept the . txt ending and everywhere in this tutorial use the actual complete file name. Even more confusing can be that many operating systems by default hide the file extension in the file browser, so that you may save a file as radius\_bending\_test.conf, and the file browser in your operating system shows it with this name, but its complete name is actually radius\_bending\_test.conf.txt. The complete name must be specified to all Numerics88 tools.

# 7.3.2 Using n88extractsets to obtain and visualize boundary conditions

Because this is a non-trivial boundary set, we really want to visualize it to make sure it is reasonable and that it corresponds to what we expect. The best way to do this is with the tool n88extractsets. This is the command to use:

n88extractsets --constraints radius82\_bending.n88model

Here "--constraints" means both boundary conditions and applied loads. (We can leave off this option, but then we will get even more output files which in the present case we are not interested in.)

The output looks like this:

```
Reading N88 Model file : radius82_bending.n88model
Writing constraint : radius82_bending_constraint_bottom_fixed.vtp
Writing constraint : radius82_bending_constraint_top_fixed.vtp
Writing constraint : radius82_bending_constraint_top_displacement.vtp
Writing constraint : radius82_bending_constraint_bottom_displacement.vtp
```

We see that four files are generated, one for each constraint. These are VTK "PolyData" files, which consist of a set of "Vertices" (points), one for each node in the boundary condition set. n88modelgenerator has separated the "fixed" constraints, which are degrees of freedom that are fixed at zero, and the "displacement" constraints, which are degrees of freedom that are fixed at zero, and the "displacement" constraints, which are degrees of freedom that are fixed at some non-zero value. This distinction is sometimes useful, although the solver does not require it. In this case the nodes belonging to the constraint or boundary condition have *x* and *y* fixed at zero, and *z* at non-zero values. Thus the "fixed" and "displacement" sets

will consist of the same set of nodes, but with different senses and values. We are going to open the file radius82\_bending\_constraint\_bottom\_displacement.vtp displacement and render it together with the contoured input image. This is shown in figure Figure 7.13. Each individual node belonging to the boundary condition is shown as a blue dot.



Figure 7.13: Set of nodes on bottom boundary condition for radius bone bending test.

### Тір

Generating this image is quite straightforward. We start with the contoured input image data, as above, then we also open the file radius82\_bending\_constraint\_bottom\_displacement.vtp, and simply render it as "Solid Color", setting the color to blue.

This looks good so we can go ahead and solve this model with faim. Expect this to take a while - go grab a coffee.

faim radius82\_bending.n88model

#### Тір

Just as in the previous model, if you have licensed the GPU solvers, and have suitable GPU hardware, then you are going to want to use it. faim can take all the arguments that n88solver can so for example:

faim --engine=nv --device=0,1 radius82\_bending.n88model

where as before the device list will depend on the number of GPUs in your system and their configuration .

As this is a very large file, once solved we should enable compression as in the previous tutorial. Compression can take a rather long time on a file this large. Remember that it is never necessary to uncompress an n88model file before reading it.

n88compress radius82\_bending.n88model

A comparison of the original input image with the solved model is shown in Figure 7.14. Here we have used a Warp By Vector filter with a Scale Factor of 15 to make the distortion more evident to the eye.



Figure 7.14: Comparison of original input and solved model of bending radius bone, with 15 times displacement amplification.

# Тір

Generating an attractive rendering of the solved model (or any n88model file) with ParaView takes a few additional steps. We saw that with an input image, we could use the Contour filter to get a nice surface with curvature that reflects the light in ways that give us visual clues about the shape of the object. An n88model file by contrast consists of a collection of cubic voxels, each of which has flat surfaces (however small they may be), all oriented the same. A direct rendering of it therefore lacks the visual lighting cues that we expect. With a few additional steps, we can convert it to a smooth surface with curvature. For Figure 7.14 we applied the following steps (to the result of the Warp By Vector filter):

- 1. Apply an Extract Surface filter. This converts the data from an Unstructured Grid (in this case a bunch of Hexahedrons) to a surface consisting of Polygons.
- 2. Apply a Smooth filter with Number of Iterations set to 300.

Another useful way to render this data is coloured by von Mises stress. See VonMisesStress. This is shown in Figure 7.15.

# Тір

You will want to manually set the scale of the coloring for von Mises stress, as the uneven contact surface has locally very high stresses, which however are uninteresting (and even unphysical, as the microscopic contact surface irregularities would yield). You can adjust the range by selecting Color Map Editor from the View menu, then click on the Rescale to Custom Range button to the left of the color map plot.



Figure 7.15: Radius in bending test with coloring by von Mises stress

Showing the von Mises stress as in Figure 7.15 is informative, but only indicates the stress on the visible surfaces. Often we will want to look at the stresses within the volume. One way to do this is with a Slice filter. This is shown in Figure 7.16. Without going into a great deal of detail, you can see the filters used in this rendering in the Pipeline Browser.

# Тір

The Slice filter should be used on volume data, and not on surface data. Notice that in Figure 7.15 we've applied the Slice filter to the output of WarpByVector1, and not to ExtractSurface1 or anything derived from it.



Figure 7.16: von Mises stress on a slice of the radius in bending test

## 7.3.3 Numerical results

The interesting quantity in the analysis file radius82\_bending\_analysis.txt (see the section on post-processing with n88postfaim) is the torque around the bending axis, which in this case is in the y direction. Refer to Figure 2.5. This quantity is given as the total of Ty in the following table from radius82\_bending\_analysis.txt. By default, this is calculated around the center of mass of the object, although you can re-run n88postfaim and specify an argument for the argument rotation\_center if you want the torques calculated around an axis passing through a different point. Because the head of the bone is "down" in the sense of smaller z, face\_z0 is the head of the bone, and face\_z1 is the cut face of the shaft. In any case, we can see that the torques balance. The numerical value of the y compenent of the torque is 1997 N·mm (see A note about units), or 1.997 N·m.

Table II: Nodal Torques							
Torque measured relative to:         60.502 94.130 48.216							
Node set: Name:				1 face_z1			
		•••••	• • • • • • • • • • • •	•••••••••••••••			
	Tx	Ту	Τz				
total	-1.213E+02	-1.997E+03	-1.928E+01				
average	-1.099E-02	-1.810E-01	-1.747E-03				
std_dev	1.134E-01	1.252E-01	2.173E-02				
minimum	-6.034E-01	-5.249E-01	-9.884E-02				
maximum	3.538E-01	4.623E-01	6.071E-02				
median	-8.431E-03	-1.915E-01	4.481E-05				

Node set: Name:				2 face_z0
• • • • • • • • • •				
	Tx	Ту	Τz	
total	1.215E+02	1.996E+03	1.927E+01	
average	1.601E-03	2.630E-02	2.538E-04	
std_dev	1.591E+00	5.163E+00	9.762E-01	
minimum	-3.176E+01	-2.068E+01	-2.480E+01	
maximum	2.722E+01	8.554E+01	2.405E+01	
median	-2.631E-02	-7.920E-01	-1.935E-02	

# 7.4 Tutorial: Radius bending with elasto-plastic material properties

In this tutorial, we are going to repeat the radius bending test of the previous tutorial, but this time we will use nonlinear elastoplastic material properties. We recommend that you first read the section on Plasticity.

# 7.4.1 Creating the model

Because nonlinear models take substantially longer to solve than linear models, for this tutorial we are going to use the reduced-resolution image file radius164.aim. However, if you have the processing power and the time to obtain solutions, and you want to use the original resolution file radius82.aim, you can of course do so.

Creating a model with elasto-plastic material properties with n88modelgenerator is straight-forward: one simply has to set the plasticity option. For example, the following configuration file is similar to the one in the last tutorial, but we have added plasticity =vonmises, 10. This means that we want a *von Mises* yield criterion (see von Mises yield criterion) with a yield strength of 10 MPa. There is no scientific justification for choosing this numerical value for the yield strength: it was chosen simply because it produces interesting results for this tutorial.

```
# File: radius_bending_elastoplastic.conf
#
# A configuration file for the tutorial: radius bending with
# elasto-plastic material properties.
input_file = radius164.aim
output_file = radius_bending_elastoplastic.n88model
test = bending
bottom_surface = visible
bottom_surface_maximum_depth = 15
plasticity = vonmises,10
```

#### As before, we generate the model with

n88modelgenerator --config radius\_bending\_elastoplastic.conf

We can verify that the resulting model file has elasto-plastic material definitions using the handy n88modelinfo command,

n88modelinfo --materials radius\_bending\_elastoplastic.n88model

#### The output is

nu : 0.3 Y : 10.0

# 7.4.2 Solving the model

We can solver the model with faim,

faim radius\_bending\_elastoplastic.n88model

Tip

As before, if you have licensed the GPU solvers, and have suitable GPU hardware, then you are going to want to use the engine and device options to obtain faster solutions.

Let us look into the file to see what fields are present for a solved elasto-plastic model. The command to list the solutions is, as before,

n88modelinfo --solutions radius\_bending\_elastoplastic.n88model

this gives an output of

Solutions:

```
Name : Solution1
Problem : Problem1
Variables defined on nodes:
Displacement
ReactionForce
Variables defined on elements:
PlasticStrain
Strain
Stress
StrainEnergyDensity
VonMisesStress
Variables defined on gauss points:
PlasticStrain
```

Everything here is as before for linear solutions, with the addition of a new field PlasticStrain. PlasticStrain is the irreversible strain that arises from exceeding the elastic limits as defined by the yield surface. See PlasticStrain in the section Calculating additional solution fields with n88derivedfields. You may also note that "variables defined on gauss points" is a new category. In essence, this is a higher accuracy version of "variables defined on gauss points", and it is required for accurately processing elastoplastic models.

### 7.4.3 Rendering yielded elements

We can use ParaView to open the solved model file radius\_bending\_elastoplastic.n88model. In Figure 7.19 we've rendered the surface of the model such that unyielded elements are shown in grey, while yielded elements are shown in red. For elasto-plastic materials, there is a clear distinction between elements that remain within the elastic limits and therefore have zero plastic strain, and those which have exceeded the elastic limits and have non-zero plastic strain. (where non-zero means that at least one of the 6 components *xx*, *yy*, *zz*, *yz*, *zx* and *xy* of the plastic strain is non-zero). In order to generate the rendering of Figure 7.19 we set the Coloring to the Magnitude of PlasticStrain. You can find these in drop-down boxes in the toolbar in ParaView, as shown in Figure 7.17. Next we will manually set a tiny range for the color scale, thus ensuring that practically

every element that is yielded is shown in fully saturated red. If we set a symmetric scale around zero, then unyielded elements, which have a PlasticStrain magnitude of zero, will be drawn in a neutral gray. To set the color scale, click the **Rescale to Custom Data Range** button, which is just to the left of the drop-down box for PlasticStrain, as shown in Figure 7.18. For this rendering I used a range of -0.00001 to 0.00001. Note that in Paraview, the Magnitude of the PlasticStrain is simply the square root of the sum of the squares of the 6 components of plastic strain. Keep in mind that this quantity has no physical interpretation, but it is useful for distinguishing yielded and unyielded elements, as here.

ParaView 4.2.0 64-bit	_ 🗆 X
<u>File Edit View Sources Filters Tools Catalyst Macros Help</u>	
😰 🖄 🐯 🗭 🔍 🗗 🧣 👢 🔣 📣 🕨 🕨 🖾 Time: 0	
📲 🎴 🛱 🛱 🖗 PlasticStrain 🔹 Magnitud 🔹 Surface 🔹 🔣 🔀 😘 茻 🗱 🛱	😫 🏼 🖉 🏵 🔾
📗 🕥 🛱 🛱 🖗 🖗 📚 🎿 😒 💫 Extract Location 🖳 🌺 💓 🛞 😽	
Pipeline Browser	

Figure 7.17: Setting the color display to the Magnitude of PlasticStrain.

_	-0-	-	-	~	<b>~</b>	•	······•	- C =	7	-	-		٣	-	-
		<b>₽</b>	<b>@</b> F	las	ticSt	rain			•	Ma	agn	itud	•		Surfa
		R	esca	le t		ustor	n Da	ta P	lan	ge	E	xtra	ct I	Lo	catio

Figure 7.18: The Rescale to Custom Data Range button.



Figure 7.19: Bending radius test with elasto-plastic material properties. Yielded elements are shown in red.

What we observe in Figure 7.19 rendering is that there are essentially three regions of plastic deformation in this bone subject to a bending force. They are,

- The uneven head of the bone. This region yields fundamentally because the deformation is applied here, and the surface is rough. Rough surfaces yield easily in localised spots: crudely speaking, you don't have to push very hard on a pointy little protusion to bend it. This yielding is uninteresting, and if you were to slice the model here, you would find that the yielding is superficial, that is, not very deep.
- On the inside surface of the bend, the bone yields in compression.
- On the outside surface of the bend, the bone yields in tension.

You can't actually tell from Figure 7.19 what is yielding in compression and what in tension, but with a little bit of more manipulation, we can generate an image that does show this. Since we know *a priori* that the tension and compression on the sides of the bone shaft will be predominantly in the *z* direction, we can change the component of YieldStrain from Magnitude to ZZ. (You may need to manually re-adjust the color scale, as ParaView will automatically rescale to the data range when you change the variable for the color.) Elements yielded in compression now show as blue, as in Figure 7.20. We have in addition used a **Slice** filter, as in the previous tutorial. This allows us to see that the yielded region is rather thick.



Figure 7.20: A slice through the radius. Yielded elements are shown in red for elements yielded in tension, and in blue for elements yielded in compression.

# 7.4.4 Numerical results

In comparison with the linear case, the y component of the torque has dropped about 1.5%, from 1.997 N·m to 1.968 N·m; hence a decrease in stiffness of 1.5%. In conclusion, this amount of plasticity has not significantly affected the results.

```
_____
Table 12: Nodal Torques
      _____
                                      60.546 94.150 48.216
Torque measured relative to:
       _____
_____
                                      _____
Node set:
                                                  1
Name:
                                              face_z1
Тх Ту
                       Τz
total -1.066E+02 -1.967E+03 -3.557E+01
average -3.555E-02 -6.560E-01 -1.186E-02
      4.106E-01 4.849E-01 7.938E-02
std dev
minimum
       -1.796E+00 -1.831E+00 -2.889E-01
maximum
       1.024E+00 1.301E+00 1.671E-01
median -3.379E-02 -6.803E-01 -2.385E-03
_____
                  _____
                              _____
Node set:
                                                  2
Name:
                                              face_z0
                           . . . . . . . . . .
        Tx Ty Tz
total1.072E+021.968E+033.570E+01average5.497E-031.009E-011.831E-03std_dev2.888E+005.542E+001.195E+00
```

## 7.4.5 A more careful calculation: incrementally applying the load

There are always more subtle considerations for nonlinear calculations than for linear calculations. One aspect of elasto-plastic calculations is that they exhibit hysteresis, or irreversible changes to strain. In this way, the solutions depend in fact, not only on the current applied state, but in principle on the whole time-dependent history.

Whether this is significant or not in practice is something that can be investigated experimentally - or rather computationally in our case. In the present case, we already know that there is only a 1.5% difference in numerical results between the linear model and the elastoplastic model. So this more careful method of applying the load in the nonlinear case is very unlikely to result in significant differences in the result. This tutorial is therefore more of a demonstration of principle, and an introduction to the possibility of modifying already-solved n88model files.

To apply the bending in increments, we will take advantage of the fact that n88modegenerator can accept an existing n88model file as input. In this case, it will preserve the grid, *i.e.* the points and elements of the model, but generate new boundary conditions and/or material definitions. Crucially, it also preserves an existing solution, which is then automatically used as the starting value when the solver is subsequently called.

We are first going to make a configuration file containing all the parameters of n88modegenerator that are the same for each increment of bending.

```
# File: common.conf
#
# A configuration file for the tutorial: radius bending with
# elasto-plastic material properties.
#
# This file contains all the parameters that don't change on
# each increment of bending.
test = bending
bottom_surface = visible
bottom_surface_maximum_depth = 15
plasticity = vonmises,10
```

Now we are going to call n88modegenerator and faim multiple times, in steps of 0.1°, from bending angle 0.6° up to bending angle 1.0°. 0.6° is chosen as a the starting angle because it happens to be just after the onset of nonlinear behaviour. In general, it takes a bit of experimentation to find the minimum applied test condition for which some elements start to exceed the linear region.

Here are the commands. You may want to put these into a script file.

```
n88modelgenerator --conf=common.conf --bending_angle=0.6 radius164.aim ↔
   incremental_bending_0.6.n88model
n88solver_sp incremental_bending_0.6.n88model
n88modelgenerator --conf=common.conf --bending_angle=0.7 incremental_bending_0.6.n88model
   incremental_bending_0.7.n88model
n88solver_sp incremental_bending_0.7.n88model
n88modelgenerator --conf=common.conf --bending_angle=0.8 incremental_bending_0.7.n88model
                                                                                             \leftarrow
   incremental_bending_0.8.n88model
n88solver_sp incremental_bending_0.8.n88model
n88modelgenerator --conf=common.conf --bending_angle=0.9 incremental_bending_0.8.n88model
                                                                                             \leftarrow
   incremental_bending_0.9.n88model
n88solver_sp incremental_bending_0.9.n88model
n88modelgenerator --conf=common.conf --bending_angle=1.0 incremental_bending_0.9.n88model
   incremental_bending_1.0.n88model
n88solver_sp incremental_bending_1.0.n88model
```

Once we have run all these commands, we can veryify that the final data file, incremental\_bending\_1.0.n88model, does indeed show the history of being processed multiple times:

n88modelinfo --history incremental\_bending\_1.0.n88model

### This gives an output of:

History: 	
2015-May-15 15:21:52 Model created by n88modelgenerator version 7.0	
2015-May-15 15:33:32 Solved by n88solver_sp 7.0	
2015-May-15 15:33:56 Model modified by n88modelgenerator version 7.0	
2015-May-15 15:50:12 Solved by n88solver_sp 7.0	
2015-May-15 15:50:36 Model modified by n88modelgenerator version 7.0	
2015-May-15 16:06:24 Solved by n88solver_sp 7.0	
2015-May-15 16:06:49 Model modified by n88modelgenerator version 7.0	
2015-May-15 16:21:46 Solved by n88solver_sp 7.0	
2015-May-15 16:22:10 Model modified by n88modelgenerator version 7.0	
2015-May-15 16:41:56 Solved by n88solver_sp 7.0	

As usual, the details can be recovered with the  $-\log option of n88 modelinfo$ , but the output is lengthy, so we will not show it here.

To perform the post-processing on the final result, we call,

```
n88derivedfields incremental_bending_1.0.n88model
n88postfaim incremental_bending_1.0.n88model
```

Numerically, the results have changed little in this case, as expected. We now have a *y*-component of torque of 1.972 N·m, which compares with 1.997 N·m in the linear case, and 1.968 N·m for the "all at once" elastoplastic case.

Table 12: Nodal Torques								
Torque measured relative to: 60.546 94.150 48.216								
Node set: Name:				1 face_z1				
total average std_dev minimum maximum median	Tx -1.109E+02 -3.700E-02 4.142E-01 -1.813E+00 9.910E-01 -4.100E-02	Ty -1.972E+03 -6.578E-01 4.917E-01 -1.875E+00 1.292E+00 -6.715E-01	Tz -4.322E+01 -1.442E-02 7.937E-02 -2.925E-01 1.608E-01 -3.440E-03					
Node set: Name:				2 face_z0				
total average std_dev minimum maximum median	Tx 1.111E+02 5.693E-03 3.203E+00 -2.743E+01 2.288E+01 -1.419E-01	Ty 1.971E+03 1.010E-01 6.189E+00 -2.847E+01 4.860E+01 -1.235E+00	Tz 4.351E+01 2.230E-03 1.350E+00 -1.076E+01 1.585E+01 2.109E-02					

This tutorial is the final tutorial in the series presenting the Faim standard workflow, with models generated by n88modelgenerator. Those interested in generating custom models will want to continue on to the tutorials presenting vtkn88. If you intend for the moment to use only n88modelgenerator for generating your models, then you can stop here.

# 7.5 Tutorial: Compressing a cube revisited using vtkn88

In the preceding tutorials, we used n88modelgenerator to quickly generate finite element models from segmented 3D images. n88modelgenerator has many parameters that can be used to tune the models in produces, but inevitably, the variety of models that can be produced using the parameter-setting approach is limited. A far more flexible approach is scripting. Numerics88 contains a collection of objects suitable for constructing and manipulating finite element objects. These can be scripted with Python. Python is one of the easiest languages to learn, and yet retains a great deal of expressive power. This collection of objects is built on top of VTK and is referred to as vtkn88. It is documented in Chapter 3.

In this tutorial, we are going to revisit the first tutorial, Introductory tutorial: Compressing a solid cube. In fact we're going to do it all over again, only this time, we will generate the model by writing a little script with vtkn88, instead of using n88modelgenerator. It will be more work, but we will have a working model-generation script that could be further tweaked to do things that would not be possible with n88modelgenerator.

# 7.5.1 Getting familiar with Python, VTK and Numpy

It is not necessary to know Python in order to write and modify scripts using vtkn88, as very often you can make obvious modifications to existing scripts. However, having a basic familiarity can make you more comfortable with the following scripting. As Python is very widely used, there are any number of excellent introductory books. A suggested place to start is the on-line tutorial at http://docs.python.org/tutorial/.

One feature of Python which we will use that is not a part of the standard Python distribution (but is distributed with Numerics88 software) is Numpy, which efficiently handles numerical arrays in Python. Again, prior knowledge of Numpy is not required, but will help. Documentation for Numpy can be found at http://docs.scipy.org/doc/. At the time of writing this manual, we recommend http://www.scipy.org/Tentative\_NumPy\_Tutorial as the best introduction.

Finally, there is VTK . VTK is quite complex and rather more difficult to learn than either Python or Numpy, but fortunately it is not necessary to know very much VTK. We will be using a mixture of custom vtkn88 objects and standard VTK objects. When one of these comes up in the following tutorials, you may want to have a glance at the corresponding API documentation for that object. This is explained in Section 3.1.

# 7.5.2 Preliminaries: first lines of Python

First create a working directory. Using your favourite text editor, create a file apply\_compression.py.

### Тір

You can also use an editor or an integrated development environment specifically intended for python, such as IDLE, but this is not necessary. A plain, old text editor will work fine. On Windows, Notepad can be used. On OS X, you can use TextEdit, which you will find in the Utilities folder within Applications. If using TextEdit, be sure to select Format  $\rightarrow$  Make Plain Text from the menu.

#### Note

If you want to cheat and not actually type this tutorial script line-by-line as we go, you can find the finished version in the Numerics88 distribution in the directory  $examples/cube_with_vtk$ .

Start by adding these lines, which import all the Python modules that we will be using:

```
from __future__ import division
import argparse
import os
import sys
import vtk
import vtkn88
```

Once you save this, you already have a script that you can run! In fact, you should run it, with just these lines in it - even though it does nothing yet, because it will verify that Python can successfully locate VTK and vtkn88. The script can be run like this (make sure you've saved cube\_compression.py),

\$ python cube\_compression.py

#### Note

The dollar sign (\$) at the beginning of the line is the prompt: don't type that. On Windows the prompt will be something like C: \>. On all systems the prompt might contain additional information, such as the current directory.

You should get as output ... nothing whatsoever. If you get an error like "ImportError: No module named vtk", then it is likely that the environment variables haven't seen set. Refer to Setting environment variables.

We recommend also having a version number in your script. Increment it whenever you change the script (not every time you add a line, but if you modify the finished script later so that the resulting model is somewhat different, then increment the version number.) We'll see soon how we can ensure that the script version number gets written into the log of the n88model file. Although we're not accountants, we highly recommend having an audit trail that will allow you to know exactly how a given model was generated. (Obviously, you should archive copies of every version of your script, not just the most recent one. You should also floss daily, which we're sure that you do.) For now, just add a version number to the script with this line (we are on version 2, since an earlier version of this manual had a slightly different implementation of this script),

 $script\_version = 2$ 

Now, we're going to want to specify the input image file on the command line, because this will allow us to use the script on any input file, not just one hard-coded by name into the script. We're also going to want to inform the user that an input file name is required if they don't supply one. ("The user" is most likely you yourself, but don't assume that next week you'll remember how you intended to use the script you write this week.) The python module argparse is really handy for this. The following lines will do the desired thing:

```
parser = argparse.ArgumentParser (
    description="""Apply a compression test.
This script does essentially the same as the command
"n88modelgenerator --test=uniaxial"
but uses VTKN88 for this purpose.
""")
parser.add_argument ("input_file",
    help="An input image file of the segmented data; must be in VTK XML format (.vti).")
args = parser.parse_args()
```

So now when we run it as before, this time we do get some output:

\$ python apply\_compression.py usage: apply\_compression.py [-h] input\_file apply\_compression.py: error: too few arguments

#### Progress!

Let's see what happens if we run it with the -h flag. Note that argparse has automatically added a -h flag, the purpose of which is to get help about the command.

```
$ python apply_compression.py -h
usage: apply_compression.py [-h] input_file
```

Apply a compression test. This script does essentially the same as the command "n88modelgenerator --test=uniaxial" but uses VTKN88 for this purpose.

positional arguments:

input\_file An input image file of the segmented data; must be in VTK XML
format (.vti).
optional arguments:
 -h, --help show this help message and exit

## 7.5.3 Reading the input file

The input file is cube6x6x6.vti and as usual you can find it in the data folder of your distribution. We've seen it before in the first tutorial. Copy it to your working directory.

As the data is in VTK's .vti format (properly referred to as "VTK XML Image Data file format"), we'll need a vtkXMLImageDataReader object to read it. That will look like this:

```
print "Reading", args.input_file
reader = vtk.vtkXMLImageDataReader()
reader.SetFileName(args.input_file)
reader.Update()
image = reader.GetOutput()
```

vtkXMLImageDataReader is a type of VTK "filter" (specifically a "source"). What we've done is very typical for VTK filters and we'll see this sequence of steps for employing a VTK filter over and over again. It is,

- 1. Create the filter object.
- 2. Set any inputs. (Here there are none, because a source doesn't have any).
- 3. Set any parameter values. In this case we set the parameter value FileName().
- 4. Call Update(). (Otherwise nothing happens and we wonder why.)
- 5. Get any output.

In fact, this isn't the only way to use VTK filter objects, but it is the simplest and it is the procedure we will nearly always employ in our scripts.

Let's provide some feedback at this point so we have some indication that the data was correctly read. While we're at it, let's do some error checking to stop things right here if that data wasn't able to be read,

```
if not image:
    print "No image data read."
    sys.exit(1)
print "Read image with dimensions", image.GetDimensions()
```

#### Now running it should result in,

\$ python apply\_compression.py cube6x6x6.vti
Reading cube6x6x6.vti
Read image with point dimensions (7, 7, 7) •

• Wait a minute! Why are the reported dimensions (7, 7, 7) when they are really  $6 \times 6 \times 6$ ? It is because these are the reported Point (or Node) dimensions, rather than the Cell (or Element) dimensions. If you're confused, review the discussion on this point in Introductory tutorial: Compressing a solid cube.

# 7.5.4 Ensuring connectivity

We could assume that the input image is properly segmented and just proceed with generating a mesh. since this is an introductory tutorial perhaps we should. However, it happens not infrequently for whatever reason that a finite element model is attempted on an image which does not consist of a single connected object. This can cause all sorts of trouble. Consider this: if there are disconnected floating bits in the model, where is the proper place for the solver to put them in the solution? Sometimes the solution of such models will be very slow, other times the model will solve OK, but some of the post-processing numbers may appear strange if you don't realize that they are calculated over the entire model, including bits which are subject to no constraints.

So to avoid potential grief, this is a good place to drop in a vtkn88ImageConnectivityFilter. It will strip away (actually zero-out) any parts of the input image that aren't in some way connected to the largest object in the image. It is a safe and prudent step in the generation of a well-defined finite element model.

```
print "Applying connectivity filter."
connectivity_filter = vtkn88.vtkn88ImageConnectivityFilter()
connectivity_filter.SetExtractionModeToLargestRegion()
connectivity_filter.SetInputData(image)
connectivity_filter.Update();
image = connectivity_filter.GetOutput() ①
```

• Wait a minute! Is it legitimate to assign the output to the variable "image" when that was also the name of the input? The answer is yes. It's quite kosher in Python to clobber a variable name by assigning it to something else. Python is more clever than you might think about this. It will in fact keep the data associated with the original "input" variable around as long required, even though we have no means to refer to it or access it now. (And technically speaking, here it will be required, at least as long as connectivity\_filter exists, because connectivity\_filter will still use the original input data. As long as connectivity\_filter is around, we might decide to use it again without changing the input, so Python won't get rid of it.)

# 7.5.5 Generating a mesh

The filter object for generating an FE mesh from an input image is vtkn88ImageToMesh. The FE mesh represents the geometry of the model, and consists of elements and nodes (concretely, it will be an object of type vtkUnstructuredGrid). Note that in VTK terminology, elements will be called Cells, and nodes will be called Points. Most of the time we don't need to set any parameters to vtkn88ImageToMesh except the input.

```
# Generate a finite element mesh from the input image
geometry_generator = vtkn88.vtkn88ImageToMesh()
geometry_generator.SetInputData(image)
geometry_generator.Update()
geometry = geometry_generator.GetOutput()
print "Generated %d elements and %d nodes." % \
        (geometry.GetNumberOfCells(), geometry.GetNumberOfPoints())
```

Now our output is beginning to get interesting,

```
$ python apply_compression.py cube6x6x6.vti
Reading cube6x6x6.vti
Read image with point dimensions (7, 7, 7)
Applying connectivity filter.
Generated 216 elements and 343 nodes.
```

Quick check:  $6^3 = 216$  and  $7^3 = 343$ , so we're good.

#### Тір

It is possible to write out the geometry to a file in VTK's XML Unstructured Grid format using vtkXMLUnstructuredGridWriter. You will then be able to open it in ParaView. It should be very similar to Figure 7.2. (In contrast though to rendering the input image, if there were any zero-valued voxels, there would be no need to threshold to remove the corresponding cells, as they are already absent from the meshed geometry.) The lines of code to save the geometry to a file are as follows:

```
writer = vtk.vtkXMLUnstructuredGridWriter()
geometry_file = "geometry.vtu"
print "Writing geometry to", geometry_file
writer.SetFileName(geometry_file)
writer.SetInputData(geometry)
writer.Write()
```

# 7.5.6 Defining materials and creating a material table

Now we need to define some material properties. We can do this by creating an instance of some specific derived class of vtkn88Material. The one of these is vtkn88LinearIsotropicMaterial. Let's make one of them,

```
print "Creating a linear isotropic material."
material = vtkn88.vtkn88LinearIsotropicMaterial()
material.SetName("linear_iso_material")
material.SetYoungsModulus(6829)
material.SetPoissonsRatio(0.3)
```

- We can give it any name we want. If we need to access it later, we can look it up by name.
- These are default values, so we actually didn't really need these lines, but it doesn't hurt be explicit, and now it is clear how to set different values should you want to do so.

The other thing we must do is to make a material table, which associates the values in the input image (segmentation IDs or material IDs) with defined materials. Our image file cube $6 \times 6 \times 6$ . vti has the uniform value of 1 on every voxel, so we need to make a material table that associates 1 with our material defined above. But perhaps we might want to run this script someday on an input file that uses different values (127 is very common for historical reasons). We could write here some fancy scripting that would examine the input data and produce a list of all the different values in the image, then map all those values to our material (since we're only using one material here). This sounds a bit complicated, but fortunately, there is a vtkn88 object, vtkn88GenerateHomogeneousMaterialTable , that does exactly this for us:

```
mt_generator = vtkn88.vtkn88GenerateHomogeneousMaterialTable()
mt_generator.SetMaterial(material)
mt_generator.SetMaterialIdList(image.GetCellData().GetScalars())
mt_generator.Update()
material_table = mt_generator.GetOutput()
print "Generated material table with %d entries." % material_table.GetNumberOfMaterials()
```

• Unfortunately, it is not as simple as just setting "image" as the argument to SetMaterialIdList. We have to be quite explicit about specifying the scalar data on the cells, in this manner.

# 7.5.7 Applying a compression test

To apply boundary conditions appropriate to a compression test, we can make use of the object vtkn88ApplyCompressionTest, which will do practically all the work for us. vtkn88ApplyCompressionTest requires as inputs both the mesh and the material table that we defined above.

```
# Apply a compression test (uniaxial)
print "Applying a uniaxial compression test."
generator = vtkn88.vtkn88ApplyCompressionTest()
generator.SetInputData(0, geometry) ①
generator.SetInputData(1, material_table) ②
generator.Update()
model = generator.GetOutput()
```

- Input 0 to vtkn88ApplyCompressionTest must be the mesh geometry, as a vtkUnstructuredGrid object.
- Input 1 to vtkn88ApplyCompressionTest must be the material table, as a vtkn88MaterialTable object.

## 7.5.8 Writing a n88model file

The output of vtkn88ApplyCompressionTest is a vtkn88FiniteElementModel object, which is a complete representation of the problem we want to solve with finite element analysis. It remains to write out this model in n88model file format.

```
# Write an n88model file
output_file = os.path.splitext(args.input_file)[0] + "_custom.n88model" 
# Remove directory, so file ends up in current directory.
output_file = os.path.split(output_file)[1]
print "Writing n88model file:", output_file
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInput(model)
writer.SetFileName(output_file)
writer.Update()
```

This is some fancy Python to derive the output file name from the input file name.

That's it. If everything works correctly, the output should look like this:

```
$ python apply_compression.py cube6x6x6.vti
Reading cube6x6x6.vti
Read image with point dimensions (7, 7, 7)
Applying connectivity filter.
Generated 216 elements and 343 nodes.
Creating a linear isotropic material.
Generated material table with 1 entries.
Applying a uniaxial compression test.
Writing n88model file: cube6x6x6_custom.n88model
```

# 7.5.9 Modifying the file history and log

We promised at the beginning to record the script version number in the file, and some far we haven't done this. First we'll have a look at what is currently in the history field.

This is useful information so instead of replacing it, we can just add to it. To do this, add the following line to the script, just before writing out the file:

model.AppendHistory("Created by cube\_compression.py version %s ." % script\_version)

Now run the script again, and this time when we run n88modelinfo, we get:

Good, now we'll always know that the cube6x6x6\_custom.n88model file was created with version 2 of the script (which called vtkn88ApplyCompressionTest from vtkn88 version 6.0).

We can also have a look at the log, which gives more detailed information:

```
$ n88modelinfo --log cube6x6x6_custom.n88model
Log:
2012-Sep-24 08:22:14
vtkn88ApplyCompressionTest settings:
TopConstraintSpecificMaterial: -1
BottomConstraintSpecificMaterial: -1
UnevenTopSurface: 0
UnevenBottomSurface: 0
TestAxis: 2
AppliedStrain: -0.01
AppliedDisplacement: 0
TopSurfaceContactFriction: 0
BottomSurfaceContactFriction: 0
ConfineSides: 0
Pin: 0
PinCellClosestToXYCenter: 1
PinCellId: 0
```

There is already quite a lot of information here, provided automatically by vtkn88ApplyCompressionTest . In particular we have all the parameters of vtkn88ApplyCompressionTest , which were all set to default values because we didn't change any of them. We could, if we wanted, add even more information to the log, using the method model.AppendLog, just as we used model. AppendHistory. In this case, there is nothing lacking that we can't query. For example, although no material information appears in the log, we can determine it with n88modelinfo,

```
$ n88modelinfo --materials cube6x6x6_custom.n88model
Materials:
Name : linear_iso_material
Type : LinearIsotropic
E : 6829.0
nu : 0.3
```

You can now proceed if you want to solve and analyze the model exactly as in An introductory tutorial: compressing a solid cube.

This completes the tutorial on building the  $6 \times 6 \times 6$  cube compression model using vtkn88. We've seen that it takes considerably more work to write a script than to call n88modelgenerator, so whenever it suffices, it is preferable to use n88modelgenerator.

However, although in this case we've done nothing that n88modelgenerator couldn't have done, we hope that you can imagine that now that we have a script, that we could potentially modify it in any number of ways beyond what would be possible with n88modelgenerator. In subsequent tutorials, we'll explore these possibilities.

# 7.6 Tutorial: Deflection of a cantilevered beam; adding custom boundary conditions and loads

In this tutorial, we are going to use vtkn88 to create a model that is different than anything that could create with n88modelgenerator. The test will be the deflection of a uniform beam fixed at one end, in other words a cantilever. We have chosen this model because there is a simple analytic solution to which we can compare the result.

One aspect that will be new to this tutorial will be an applied force as part of the problem definition. Generally though, it is preferable to define models with fixed position boundary conditions and solve for the forces, rather than to specify forces and solve for a displacement. The reason for this will be discussed in the subsequent tutorial.

The completed script, create\_cantilever.py, can be found in the cantilever subdirectory in the examples.

### 7.6.1 Importing the required python modules

As in the previous tutorial, we start the python script by importing the python modules that we will need. This time we will also need the numpy module, as we are going to do some array manipulation.

```
from __future__ import division
import argparse
import numpy
from numpy.core import * 
import vtk
import vtkn88
from vtk.util.numpy_support import vtk_to_numpy, numpy_to_vtk
```

- This just saves some typing later. For example we'll be able to use the function array instead of the longer numpy. array.
- **2** These are the functions that allow us to convert numpy arrays to and from VTK data arrays.

As before, we'll also set a script version number:

 $script_version = 2$ 

### 7.6.2 Setting command line options

As before, we use the argparse module, which makes it quite simple to define a couple of arguments for running the script, one of which, the applied force, will have a numerical value.

```
parser = argparse.ArgumentParser (
    description="""Generate a model for a cantilever with an
applied force to the end of the beam.""")
parser.add_argument ("applied_force", type=float,
    help="The applied force to the end of the beam.")
parser.add_argument ("output_file",
    help="Name for output n88model file.")
args = parser.parse_args()
```

# 7.6.3 Generating the image data

The beam is going to have a very simple geometry, one which we generate algorithmically without too much trouble. This is also going to serve as a brief introduction to numpy arrays. Because the analytic solution for the cantilever is essentially a 2D problem, we are going to use just a beam width of just a single element. To scale up to a realistic width, if desired, one can just scale all the forces. We are going to create a beam of  $200 \times 1 \times 20$  elements, with a cubic element of side length 0.5mm. Thus the beam has dimensions of length 100mm, height 10mm, and width 0.5mm (but again, everything scales linearly with the width, so the obtained solution can be used for arbitrary widths).

Here is how we create a 3-dimensional array data of size  $200 \times 1 \times 20$ :

```
dims = array ((20, 1, 200)) ①
cellmap = ones (dims) ②
```

- The order of the dimensions is z,y,x, because numpy indices always are ordered with the "fastest-changing" index last, which must be x. On the other hand, VTK will generally want arguments specified as x,y,z. We will have to be careful about which order to use when.
- ones is a numpy function that creates an array (in this case a 3-dimensional array) filled with 1s.

We to convert this from a numpy array, which is natural to Python, to to a VTK data array:

```
cellmap_vtk = numpy_to_vtk(ravel(cellmap), deep=1, array_type=vtk.VTK_INT)
```

There are a couple of subtle points here. The first is that VTK is actually going to want the flattened data, meaning as one long 1-dimensional array, rather than as a 3-dimensional array. (It will keep track of the dimensionality separately, as we will see below.) Hence the use of ravel function, which is a numpy function that returns the input array as a one-dimensional array (without copying the underlying data if possible). The other aspect to note is that we specify deep=1, which specifies that the VTK array should create its own copy of the underlying data, instead of just referring to the numpy data. This is less memory efficient, but there are potential pitfalls with sharing the data, so we'll go with the more robust method of making a copy.

Now that we have the data, we're going to create a vtkImageData object which adds information such as the dimensions and the spacing.

```
image = vtk.vtkImageData()
image.SetDimensions(dims[::-1] + 1) 
image.SetSpacing(0.5, 0.5, 0.5)
image.GetCellData().SetScalars(cellmap_vtk)
```

This is a little bit tricky. First,  $\dim s[::-1]$  simply means "dims reversed", which we need because, as discussed above, dims is ordered *z*,*y*,*x*, but VTK requires *x*,*y*,*z*. Secondly we're adding 1 (to every dimension) because vtkImageData dimensions are always in terms of the number of Points, rather than the number of Cells.

We've set the spacing to 0.5. In this tutorial, we are going to use units of millimetres. Units are not specified in the n88model file. Instead we will just have to ensure that all our units are consistent. See A note about units.

We can at this point write out the vtkImageData as a .vti file, and open it with ParaView to ensure that we have obtained the desired result. It should ressemble Figure 7.21. As a beam, it looks absurdly thin, but to emphasise once again, we are solving essentially a 2D problem; the numerical results obtained can be scaled to any beam width.

```
# Optional: write out image data to examine it
print ("Writing geometry file: beam_image.vti")
writer = vtk.vtkXMLImageDataWriter()
writer.SetInputData(image)
writer.SetFileName("beam_image.vti")
writer.Update()
```



Figure 7.21: Generated beam image.

# 7.6.4 Generating a base model without boundary conditions

Now that we have an image, as in the previous tutorial, we convert it to a geometric mesh:

```
# Generate a geometrical mesh from the input image
mesh_generator = vtkn88.vtkn88ImageToMesh()
mesh_generator.SetInputData(image)
mesh_generator.Update()
mesh = mesh_generator.GetOutput()
```

### We also define a material (steel) and a material table.

```
# Create a material
material = vtkn88.vtkn88LinearIsotropicMaterial()
material.SetName("steel")
material.SetYoungsModulus(2.0E5) ①
material.SetPoissonsRatio(0.3)
material_table = vtkn88.vtkn88MaterialTable()
material_table.AddMaterial (1, material) ③
```

- 200GPa is a typical value for the Young's modulus of steel. We will use units of MPa. We have already declared that our length units are mm, hence all units will be consistent provided that we use Newtons for forces.
- The value 1 comes from the fact that we filled our image with 1s. All the elements will now be mapped to the material "steel".

In contrast to the previous tutorial, we won't be using one of the standard test generation filters. Rather we will use the base test generation filter vtkn88ApplyTestBase, which creates a vtkn88FiniteElementModel object without any boundary conditions.

model = generator.GetOutput()

```
# Create a model without boundary conditions.
generator = vtkn88.vtkn88ApplyTestBase()
generator.SetInputData(0, mesh)
generator.SetInputData(1, material_table)
generator.Update()
```

Before we add displacement boundary conditions and applied loads, let's save the model so we can examine the results as we build up our script. Of course the model isn't complete yet, but that doesn't prevent us from saving and examining it.

```
# Write an n88model file
print "Writing n88model file:", args.output_file
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInputData(model)
writer.SetFileName(args.output_file)
writer.Update()
```



#### Important

In everything that follows, it is intended that you add new lines to the script **before** the code (shown just above) that saves the model to a file. Otherwise of course the saved file won't include our additions and changes.

To run the script will require both a numerical value for the applied force and an output file name. For now use these values:

```
python create_cantilever.py -10 cantilever.n88model
```

We are choosing to use a negative applied force, because it is more natural to think of a downward force applied to a cantilever.

### 7.6.5 Adding fixed boundary conditions

We want to fix one end of our beam, to weld it to the (virtual) wall. Usually the step requiring the most work in defining boundary condition is identifying the set of nodes that constitute the boundary surface we are interested in. In this case, vtkn88ApplyTestBase has done the work for us, because although it doesn't define any boundary conditions, it does define node (and element) sets on all the faces. (To be more precise, it defines node and element sets consisting of any nodes/elements located at the *x*, *y* and *z* extents of the model.) This is discussed in Creating node and element sets. The names of these sets are listed there, but if you've run the script up to this point, you can also use n88modelinfo to query the set names:

```
Part : Part1
NumberOfNodes : 42
Name : face_y0
Part : Part1
NumberOfNodes : 4221
Name : face_y1
Part : Part1
NumberOfNodes : 4221
```

There are also corresponding element sets, which can be listed with the --element\_sets option to n88modelinfo.

Node set "face\_x0" is the one to which we are interested in applying a fixed boundary condition. If you refer to the the API documentation for vtkn88FiniteElementModel, you will see that there are a number of methods for defining boundary conditions. One possibility is to use the method FixNodes, which will fix the specified node set in all senses (directions). Only one line of code would be required:

model.FixNodes ("face\_x0", "fixed\_beam\_base")

• "face\_x0" is the name of an existing node set; "fixed\_beam\_base" is the name we are assigning to the new constraint.

However, as we are trying to obtain a result as close as possible to the analytic 2D solution, it is actually better to not to limit the freedom of motion in the *y* direction on the boundary condition. This way, no *y* direction forces will arise. Were there to be any forces in the *y* direction, this would cause some essentially 3D effect on the *x*-*z* plane by the mechanism of Poisson's ratio. So instead of using FixNodes, we will use the following slightly more verbose code

```
# Create the fixed boundary conditions at the base of the beam.
# To obtain a more truly 2D result, no constraint is applied to
# displacements in the _y_ direction.
model.ApplyBoundaryCondition(
    "face_x0",
    vtkn88.vtkn88Constraint.SENSE_X,
    0,
    "fixed_beam_base_x")
model.ApplyBoundaryCondition(
    "face_x0",
    vtkn88.vtkn88Constraint.SENSE_Z,
    0,
    "fixed_beam_base_z")
```

If you now run the script, you can then use n88modelinfo to verify that the boundary condition has indeed been generated:

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## 7.6.6 Adding an applied load to tip of the beam

At the free end of the beam, we are going to apply a load. Creating an applied load is very similar to creating a displacement boundary condition. vtkn88FiniteElementModel provides a number of methods for this purpose. There are some important differences,

- 1. Applied loads are applied to element sets; displacement boundary conditions are applied to node sets.
- 2. Applied loads require the additional specification of a particular face of the elements to which to apply the load, or else the specification that it is a body force. We are going to apply the load to the outward faces of the end elements (*i.e.* in the *x* direction).

Here is the code to create an applied load constraint, named "end\_force" to the pre-defined element set "face\_x1". corresponding to the end face of the beam.

```
# Apply a force to the far end of the beam
model.ApplyLoad(
    "face_x1", ①
    vtkn88.vtkn88Constraint.FACE_X1_DISTRIBUTION, ②
    vtkn88.vtkn88Constraint.SENSE_Z, ③
    args.applied_force, ④
    "end_force") ⑤
```

- This node set was created by vtkn88ApplyTestBase . Here "face\_x1" means elements on the x1 face of the entire model.
- <sup>2</sup> This specifies the *x1* faces of the elements.
- This specifies the direction of the applied force. (The value of vtkn88.vtkn88Constraint.SENSE\_Z is 2, but the named constant conveys the intent more clearly than the numerical value.)
- The applied force will be equally divided among the element faces in the set. Units, as discussed above, are Newtons.
- 5 The name of the newly-created constraint.

## 7.6.7 Specifying sets for post-processing

There is one more step required, and that is to identify the sets to be used for post-processing calculations by n88postfaim. We are interested in values on the sets "face\_x0" and "face\_x1". The magic lines of code are:

```
# Set the node sets and element sets that will be used for post-processing
```

```
info = model.GetInformation()
pp_node_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_NODE_SETS()
pp_elem_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_ELEMENT_SETS()
pp_node_sets_key.Append(info, "face_x0")
pp_elem_sets_key.Append(info, "face_x1")
pp_elem_sets_key.Append(info, "face_x1")
```

After running the script, we can verify that these post-processing sets are in fact specified in the n88model file:

```
$ n88modelinfo --problems cantilever.n88model
Problems:
Name : Problem1
Part : Part1
Constraints : fixed_beam_base_x,fixed_beam_base_z,end_force
PostProcessingNodeSets : face_x0,face_x1
PostProcessingElementSets : face_x0,face_x1
```

#### Tip

It is possible to skip this step, and instead to specify later the node and element sets to be used by n88postfaim on the command line of n88postfaim with the argument

```
--sets=face_x0,face_x1
```

# 7.6.8 Documenting the model in the file log

As discussed previously, it is good practice to document the model creation in both the file History and the file Log. Here we add these lines (again they must come before the code that saves the model):

```
# Update history and log
model.AppendHistory("Created by create_cantilever.py version %s ." % script_version)
model.AppendLog(
"""create_cantilever.py
Cantilever beam model with applied force on far face of %s .
Using VTKN88 version %s .
""" % (args.applied_force, vtkn88.vtkn88Version.GetVTKN88Version()))
```

If we run the script to generate the n88model file, we can at any later time get a brief description of the model and determine what versions were used (including what version of vtkn88).

### 7.6.9 Solving the problem and comparing with theory

The model is quickly solved with faim:

```
$ faim cantilever.n88model
```

If we open the solved file cantilever.n88model in ParaView, we can observe the beam deflection as shown in figure Figure 7.22. Here the deflection is amplified by 10 so as to be more evident. The figure is colored by the *xx* component of strain, with red being tensile and blue being compressive. This is easily done in ParaView, simply by selecting the relevant quantities from the drop-down boxes in the toolbar, as in figure Figure 7.23.



Figure 7.22: Deflection of loaded cantilever beam. Displacement amplified by 10. Coloration by xx component of strain.

	¥¥	<b>-</b> )	(4	C.	f		<b>⊮</b>		11				÷.	şП	me:	U			_
	<b>†</b> ℃	🥡 S	traiı	۱				•	хх			•	Sur	face			•	X	P
			Ø		<u></u>	~	0	°		E>	trac	t Lo	ocati	on		0	ALERT	0	



Now let's compare quantitatively with the analytical result for deflection of a cantilever beam as found in any Mechanics of Solids textbook or on wikipedia at https://en.wikipedia.org/wiki/Deflection\_%28engineering%29 ). We have that the deflection  $\delta$  of the end of a cantilever beam is

$$\delta = \frac{FL^3}{3EI}$$

where

F	= force acting on the tip of the beam
L	= length of the beam (span)
Е	= modulus of elasticity
Ι	= area moment of inertia

For a beam with a rectangular cross-section  $b \times h$ , the area moment of inertia is

$$I = \frac{bh^3}{12}$$

so that we have

$$\delta = \frac{4FL^3}{Ebh^3} = \frac{4(10\,\text{N})(100\,\text{mm})^3}{(2 \times 10^5\,\text{MPa})(0.5\,\text{mm})(10\,\text{mm})^3} = 0.4\,\text{mm}$$

You can observe this deflection in ParaView, and we can get a precise number by looking in the beam\_analysis.txt file, in the table "Nodal Displacements". In this case the result, 0.4018, is very close to 0.4.
Node set:		1
Name:		face_x0
	ux uy uz	
average	0.000E+00 -7.848E-19 0.000E+00	
std_dev	0.000E+00 3.690E-05 0.000E+00 0.000E+00 _7 268E-05 0.000E+00	
maximum	0.000E+00 7.268E-05 0.000E+00	
median	0.000E+00 6.948E-12 0.000E+00	
Node set:		2
Name:		face_x1
• • • • • • • • • •		••••••
average	2,795F-09 -4,568F-19 -4,018F-01	
std_dev	1.812E-02 7.627E-07 1.070E-05	
minimum	-2.997E-02 -1.124E-06 -4.018E-01	
maximum	2.997E-02 1.124E-06 -4.018E-01	
imum imum ian	-2.997E-02 -1.124E-06 -4.018E-01 2.997E-02 1.124E-06 -4.018E-01 -1.860E-08 2.091E-08 -4.018E-01	

Figure 7.24: Amount of deflection of the end face of the cantilever beam, as found in the analysis file.

This concludes the cantilever beam tutorial. We learned how to create custom models using vtkn88 that are beyond the standard types of models that n88modelgenerator can generate. We were also introduced to a new type of constraint, which was the applied load.

# 7.7 Tutorial: A cantilevered beam with elastoplastic material properties

This tutorial uses the same model as the previous one, but now we will solve it using nonlinear elastoplastic material properties.

## 7.7.1 Analytic solution

The cantilever problem has a known analytic solution even in the case of nonlinear elastoplastic material properties. This solution is due to Timoshenko and Gere (1997).

Before building and solving some models, we will consider the analytic solution, because it will indicate what range of test loads are both interesting and reasonable, which is a non-trivial question for nonlinear problems.

The applied load at which the cantilever begins to yield, Fy, is

$$F_y = \frac{\sigma_y b h^2}{6L}$$

where  $\sigma_y$  is the material yield strength (*i.e.* the value of uniaxial stress at which the material starts to yield), and all other symbols are as in the previous section.

For our current model, for which we will use  $\sigma_y = 120$  MPa, this evaluates to

$$F_y = \frac{(120 \text{ MPa})(0.5 \text{ mm})(10 \text{ mm})^2}{6(100 \text{ mm})} = 10 \text{ N}$$

You will notice that this value is corresponds (not entirely coincidently) with the applied force used for the linear case in the previous section, for which we had calculated a deflection of 0.4 mm.

In the yielding region, the beam deflection is

$$\frac{\delta}{\delta_y} = \left(\frac{F_y}{F}\right)^2 \left(5 - \left(3 + \frac{F}{F_y}\right)\sqrt{3 - \frac{2F}{F_y}}\right)$$

This expression is only valid for  $1 \le F / F_y \le 3/2$ ; the cantilever will not withstand any force larger than this. For the current model this range corresponds to between 10 N and 15 N.

### 7.7.2 Changes to the generation script

The model generation script is named create\_cantilever\_ep.py. It differs from the script in the previous tutorial, create\_cantilever.py, only in the definition of the material. This becomes

```
# Create a material
material = vtkn88.vtkn88VonMisesIsotropicMaterial()
material.SetName("steel")
material.SetYoungsModulus(2.0E5)  # units are MPa
material.SetPoissonsRatio(0.3)
material.SetYieldStrength(120)  # units are MPa
```

For a *von Mises* elastoplastic material, we have exactly one new parameter as compared with a linear material, and that is the yield strength, here set to 120 MPa. The exact parameters required depend on the material. For example a *Mohr Coulomb* material would have two additional parameters, which are set with the method SetYieldStrengths(Y\_tension, Y\_- compression). As always, for exact usage refer to the vtkn88 API documentation (vtkn88VonMisesIsotropicMaterial and vtkn88MohrCoulombIsotropicMaterial).

# 7.7.3 Plastic strain distribution

One note about solving this model: the cantilever is, for various reasons, a particularly difficult model for a finite element solver. When combined with nonlinear material properties, in order to get the most accurate results, it is necessary to tighten the convergence tolerance. Thus for the following results, we ran the solver as follows,

```
faim --conv=1E-9 cantilever_ep.n88model 0
```

The complete argument is --convergence\_tolerance, but --conv also works because it is unambigous: no other option starts with the same four letters.

### Тір

Although this is a small model, elastoplastic models take considerably longer to run than linear models, so if you have a system with a suitable GPU, make use of the option --engine=nv. On the other hand, such a small model is solved fastest all on one GPU, even in a system with multiple available GPUs.

A solution with applied force of 14.5 is shown in figure Figure 7.25. In comparison with the linear case of figure Figure 7.22, we see that the strain is much more concentrated near the fixed end of the beam.



Figure 7.25: Deflection of loaded elastoplastic cantilever beam. Displacement amplified by 10. Coloration by xx component of total strain.

# 7.7.4 Comparison of finite element and analytic results

By generating and solving models for various loads in the plastic range, we can generate table Table 7.1. Explicitly, we run the following commands:

```
python create_cantilever.py -10 cantilever_ep_100.n88model
faim --conv=1E-9 cantilever_ep_100.n88model
python create_cantilever.py -10.5 cantilever_ep_105.n88model
faim --conv=1E-9 cantilever_ep_105.n88model
python create_cantilever.py -11 cantilever_ep_110.n88model
faim --conv=1E-9 cantilever_ep_110.n88model
```

and so on . . .

As we can see from the number of elements exceeding the plastic limit (the last column of the table), FAIM does indeed show plastic onset at 10 N load. The data are visualized in table Figure 7.26. Agreement is very good until the onset of beam failure approaches. Then there begins to be a some divergence between FAIM and the analytic results. Better agreement can be obtained with a smaller element size, but fundamentally near the singularity of failure, there are very rapid changes in plastic strain through the cross-section, and these cannot be well modelled by numerical discretisation. However, away from this singularity, numerical results are good.

### Tip

When running several models at different parameter points, it can become tedious to open each analysis file and search out the relevant quantity. We can use the n88tabulate tool to save some effort. In the present case, after we have solved all the models, the following command will generate the 4<sup>th</sup> column of the table (displacement as calculated by FAIM):

n88tabulate -V dz\_avg\_ns2 \*\_analysis.txt

The variable name for the desired quantity (here  $dz_avg_ns2$ ) can either be found in the n88tabulate section of the manual, or by referring to the on-line help from running n88tabulate with the -h flag.

load	linear	analytic EP	FAIM EP	plastic elems
10.0	0.40	0.4000	0.4020	2
10.5	0.42	0.4201	0.4222	4
11.0	0.44	0.4406	0.4427	28
11.5	0.46	0.4621	0.4641	50
12.0	0.48	0.4852	0.4869	84
12.5	0.50	0.5107	0.5120	124

Table 7.1: Elastoplastic cantilever results

load	linear	analytic EP	FAIM EP	plastic elems
13.0	0.52	0.5397	0.5404	174
13.5	0.54	0.5745	0.5738	228
14.0	0.56	0.6188	0.6149	294
14.5	0.58	0.6835	0.6700	368
15.0	0.60	0.8889	0.7560	454
15.5	0.62	_	0.9611	556



Figure 7.26: Comparison of FAIM and analytic results for elastoplastic cantilever.

### Tip

If you want, you can experiment with increasing the number of elements in the model (reducing the element size) to see how this affects the result.

# 7.7.5 Incremental loading and hysteresis

Up to this point, we have solved a sequence of nonlinear models at different loads without giving a lot of thought about how these loads are applied. In fact we have solved each load point "from scratch". From a theoretical point of view, it would be better to start from the greatest load for which the model stays in the linear range, and then incrementally add small amounts of load, obtaining a sequence of slowly changing nonlinear solutions, each of which is used as the starting point for the solver for the subsequent load. This is discussed in Obtaining accurate nonlinear solutions by progressively applying loads. The question is, does this actually matter? Here we will investigate this and discover that the answer is "it depends".

The first thing we need is a script to take an existing solved n88model file, and modify the applied force. You can find this script, named modify\_force.py, in the cantilever subdirectory of the examples. Since you are getting by now pretty good at scripts, here are all the preliminaries, up to reading in an existing n88 model file:

```
from ___future__ import division
import argparse
import vtk
import vtkn88
script\_version = 1
parser = argparse.ArgumentParser (
    description="""Take an existing cantilever model file, and modify the applied force
while leaving any existing solution unmodified. It can thus be used as the starting
value for a solution with the new applied force.""")
parser.add_argument ("input_file",
  help="An existing cantilever model file.")
parser.add_argument ("applied_force", type=float,
  help="The new applied force.")
parser.add_argument ("output_file",
   help="Name for output file.")
args = parser.parse_args()
# Read existing model (including possible solution)
print "Reading n88model file:", args.input_file
reader = vtkn88.vtkn88N88ModelReader()
reader.SetFileName (args.input_file)
reader.Update()
model = reader.GetOutput()
```

Now, we could modify the numerical values of the force constraint, but from a programming view, it is easier to just delete it and re-create it.

```
# Delete the old applied force.
model.GetConstraints().RemoveItem("end_force")
# Apply the new force to the far end of the beam.
model.ApplyLoad(
        "face_x1",
        vtkn88.vtkn88Constraint.FACE_X1_DISTRIBUTION,
        vtkn88.vtkn88Constraint.SENSE_Z,
        args.applied_force,
        "end_force")
```

That's the meat of it. Now we just finish up with the usual entires to the history and the log, and write out the modified file.

```
# Update history and log
model.AppendHistory("Modified modify_force.py version %s ." % script_version)
model.AppendLog(
"""modify_force.py
Changed applied force on far face edge to %s .
Using VTKN88 version %s .
""" % (args.applied_force, vtkn88.vtkn88Version.GetVTKN88Version()))
# Write an n88model file
```

```
print "Writing n88model file:", args.output_file
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInputData(model)
writer.SetFileName(args.output_file)
writer.Update()
```

### Tip

Had we created the model with n88modegenerator, it would have been even easier to change the load in the model file: n88modegenerator can take as an input an existing model file, and it will preserve any existing solutions while modifying the material properties or constraints according to the command line arguments in the usual fashion.

Now to run this, we first create and solve a nonlinear model as we did above, with an applied force that we know, from the previous analysis, is just at the limit of linear behaviour.

```
python create_cantilever_ep.py -10 cantilever_ep.n88model
faim --conv=1e-9 cantilever_ep.n88model
```

As previously, we can extract from the analysis file just the numerical value for the deflection, like this

```
n88tabulate -V dz_avg_ns2 cantilever_ep_analysis.txt
```

which returns -4.020E-01.

Now we use our modify\_force.py script to increase to applied force to -10.5.

python modify\_force.py cantilever\_ep.n88model -10.5 from\_100\_to\_105.n88model

And we solve it and extract the new deflection.

faim --conv 1E-9 from\_100\_to\_105.n88model

What we want to see, is that faim starts with the following two status lines:

```
Model contains elastoplastic material definitions.
Model contains existing solution.
```

And further on, once the solver solver\_sp itself has been launched, we want to verify that we see the following status output:

Using existing solution as starting value.

#### Then, rinse and repeat until the desired final load is reached:

```
python modify_force.py from_100_to_105.n88model -11 from_105_to_110.n88model
faim --conv 1E-9 from_105_to_110.n88model
n88tabulate -V dz_avg_ns2 from_105_to_110_analysis.txt
python modify_force.py from_105_to_110.n88model -11.5 from_110_to_115.n88model
faim --conv 1E-9 from_110_to_115.n88model
n88tabulate -V dz_avg_ns2 from_110_to_115_analysis.txt
```

and so on . . .

We can thus add another column to Table 7.1, and compare the "all-at-once" nonlinear solutions with the incremental solutions. Table 7.2 shows just these two columns. The results are practically indistinguishable. So can we therefore conclude that carefully applying an incremental load is pointless extra work? Not quite. We are not at the end of the story yet. Let us take our solution at a load of 14.5, and from there *decrement* the applied load back down to the linear region. Programmatically, this looks much like before:

```
python modify_force.py from_140_to_145.n88model -14 from_145_to_140.n88model
faim --conv 1E-9 from_145_to_140.n88model
python modify_force.py from_145_to_140.n88model -13.5 from_140_to_135.n88model
faim --conv 1E-9 from_140_to_135.n88model
```

and so on . . .

We can tabulate all the deflections at once,

n88tabulate -V filename,dz\_avg\_ns2 \*\_analysis.txt

These additional load decreasing points are tabulated in Table 7.3. These are plotted together with the increasing load points up to 14.5 in Figure 7.27. Now we see that that there is in fact a difference. Indeed we recognize the classic hysteresis curve. (Note that compared with Figure 7.26, we have swapped the axes, just so that it looks more conventional.)

load	FAIM EP	FAIM incr
10.0	0.4020	0.4020
10.5	0.4222	0.4222
11.0	0.4427	0.4427
11.5	0.4641	0.4641
12.0	0.4869	0.4870
12.5	0.5120	0.5120
13.0	0.5404	0.5405
13.5	0.5738	0.5738
14.0	0.6149	0.6150
14.5	0.6700	0.6700
15.0	0.7560	0.7560
15.5	0.9611	0.9611

Table 7.2: Elastoplastic cantilever incremental results

load	FAIM decr
14.0	0.6499
13.5	0.6299
13.0	0.6098
12.5	0.5897
12.0	0.5696
11.5	0.5495
11.0	0.5294
10.5	0.5093
10.0	0.4892
0.0	0.0874

Table 7.3: Elastoplastic cantilever results for decreasing loads



Figure 7.27: Hysteresis exhibited by elastoplastic cantilever.

This concludes the tutorial on a cantilever with elastoplastic material properties. We learned how to use elastoplastic materials in VTKN88 scripts, and also how to apply loads incremental steps to nonlinear models by modifying an existing n88model file. By carefully applying incremental loading to the cantilever, we determined that results were essentially unaffected as compared with an "all at once" solution for the initial deflection of the beam, but that a residual deflection remains during the subsequent unloading of the beam. This residual deflection, which is the hysteresis, can only be observed by applying the load incrementally.

# 7.8 Advanced custom model: A screw pull-out test

In the preceding tutorials we were introduced to using vtkn88 to create original models that cannot be generated using n88modelgenerator. We mentioned that frequently the most challenging part of creating such models is identifying the sets of nodes and/or elements corresponding to the boundary conditions that we desire. In that tutorial, however, we didn't actually need to identify any such sets ourselves, as we found that the standard node and element sets as provided by vtkn88ApplyTestBase were suitable for our purposes. In this tutorial, by contrast, we will use some sophisticated criteria for identifying the desired sets for boundary conditions. This includes,

- Identifying and characterizing features in the input image. Namely, we will determine the geometric location of a screw axis.
- Identifying nodes by spatial location (distance from the screw, as well as depth from the top surface).
- We will further reduce the selection of nodes based on visibility from a certain viewing angle, which is a useful technique for locating nodes on an uneven surface.

In the course of this example, we will generate the files screwpullout.py and screwpullout.conf. You can find the completed versions of these files in the examples/screwpullout directory of the distribution.

# 7.8.1 The model: a screw pull-out test

This example is a finite element model of an important mechanical test for orthopaedic biomechanics. This tutorial is based on the work of Stadelmann et al (2012). Physical tests were done in which a volume of bone substitute was constrained with a ring and the screw was pulled out. Here we construct a finite element model corresponding to this physical test.

The geometry of the model is in the file sawbone.aim in the data directory of the distribution. It consists of a volume of bone substitute into which a screw has been embedded. This is shown in Figure 7.28. The data have been segmented such that bone substitute is labelled with ID 127 (shown in beige), and the screw with ID 90 (shown in blue). The mechanical test is to find the force required to pull out the screw.



Figure 7.28: Screw model segmented image

# **!**

# Important

The script will look for the data file sawbone.aim in whatever directory it is run from. On your distribution, the example script and the data file are in different directories, examples/screwpullout and data respectively. We recommend that you copy the files from both these directories to a temporary working directory for this tutorial.

### 7.8.2 Preliminaries: first lines of Python

Using your favourite text editor, create a file screwpullout.py.

By now you should be pretty familiar with importing the necessary Python modules:

```
from __future__ import division
import os
import sys
import time
import vtk
import vtkn88
```

As before, we'll also set a script version number:

script\_version = 6 ①

#

• A version of this script has been used as a tutorial in previous versions of Faim. In Faim 7.0 we are on the 6<sup>th</sup> iteration of this script.

Since generating a model from a large micro-CT scan can take a lot of time, it is convenient to print status messages as the script proceeds, and to have these messages time stamped, so that we can see what steps potentially should be optimized (or where the script fails). The following function will take one or more strings and print them out one per line, with a time stamp on the first, and indenting the subsequent lines.

```
def message(msg, *additionalLines):
    """Print message with time stamp.
    The first argument is printed with the a time stamp.
    Subsequent arguments are printed one to a line without a timestamp.
    """
    print "%8.2f %s" % (time.time()-start_time, msg)
    for line in additionalLines:
        print " * 9 + line
    start_time = time.time()
```

## 7.8.3 Using a configuration file to store parameters

This model is going to be quite complicated. To keep things orderly, we will put all our parameters in a configuration file. The configuration file is a record of exactly which parameters were used to generate a particular model. We're going to write the configuration file itself in Python code, so that we don't have to write a file parser to read it. Here is what the configuration file (screwpullout.conf) looks like:

```
# Configuration file screwpullout.conf
#
# This configuration file is in the format of python source code.
# If you stick with simple assignments, then it looks like a typical
# configuration file, and can probably be read with other file parsers,
# if you wish to do so.
# Input image file.
input_image_file = "sawbone.aim"
# Output n88model file.
# - take the input file name and change the extension to .n88model
n88model_file = os.path.splitext(input_image_file)[0] + ".n88model"
# Bone material
```

```
bone_material_id = 127
bone_material_modulus = 6829.0
                                 # 6829.0 MPa for bone
bone_material_poissons_ratio = 0.3
# Screw material
screw_material_id = 90
screw_material_modulus = 69000.0
                                 # 69 GPa for Aluminum
screw_material_poissons_ratio = 0.3
# Displacement (in physical length units of the model) applied to the screw
# surface.
screw_displacement = 0.01
# Ring radii for finding nodes of bone material to which we will apply the
# constrained ring.
inner_ring_radius = 4.5
outer_ring_radius = 7.0
# Max depth for finding nodes of bone material to which we will apply the
# constrained ring. The max is measured from the highest node of constrained
# bone found.
bone_constraint_max_depth = 1.5
```

Now we add to our script the following:

- 1. A bit of code to get the configuration file name from the command line.
- 2. One line to execute the configuration file as Python code.
- 3. Some lines to print out all the values that we expected to read in. This is very good practice so when you run it, you can verify that everything is as you expect.

All that looks like this:

```
if len(sys.argv) != 2:
  print "Usage: python screwpullout.py example.conf"
  sys.exit(1)
config_file = sys.argv[1]
# Read in configuration file.
message("Reading configuration file " + config_file)
# Here we are actually executing it as python code.
execfile(config_file)
# Print out values that we read in. This also has the effect of causing
# this script to die if configuration values are missing (which is a good thing).
settings_text = ["Configuration:"]
settings_text.append( "input file
                                                      = %s" % input_image_file)
settings_text.append( "output file
                                                      = %s" % n88model_file)
settings_text.append( "bone material id
                                                      = %s" % bone_material_id)
settings_text.append( "bone material Young's modulus = %s" % bone_material_modulus)
settings_text.append( "bone material Poisson's ratio = %s" % bone_material_poissons_ratio)
settings_text.append( "screw material id
                                                      = %s" % screw_material_id)
settings_text.append( "screw material Young's modulus = %s" % screw_material_modulus)
settings_text.append( "screw material Poisson's ratio = %s" % screw_material_poissons_ratio ↔
   )
settings_text.append( "screw displacement
                                                      = %s" % screw_displacement)
settings_text.append( "inner ring radius
                                                      = %s" % inner_ring_radius)
settings_text.append( "bone constraint max depth
                                                      = %s" % bone_constraint_max_depth)
message(*settings_text) ①
```

• This is slightly advanced python, where the asterisk means that we pass the list of N items (strings in this case) not as a single list argument, but as N individual arguments. It just happens that given the way we wrote our message function, this is the best thing to do here.

Now when we run our script, we also have to specify the name of the configuration file:

```
$ python screwpullout.py screwpullout.conf
```

## 7.8.4 Reading the segmented image file

We will use a vtkn88AIMReader to read the data file, which is in the Scanco AIM file format. This file contains a segmented image. As well, we want to add some additional lines to report our progress, and print some values as a sanity check.

```
message("Reading input data.")
reader = vtkn88.vtkn88AIMReader()
reader.SetFileName(input_image_file)
reader.DataOnCellsOn() 
reader.Update()
image = reader.GetOutput()
message("Read %d points from image file." % image.GetNumberOfPoints())
image_bounds = image.GetBounds() 
message("Image bounds:", (" %.4f"*6) % image_bounds)
```

- As discussed in several previous tutorials, we can either have the image data on the Cells or the Points. vtkn88 is generally agnostic on this point, but it is good to be clear.
- This is a standard VTK method for many types of VTK objects, returning an array of six values:  $x_{min}$ ,  $x_{max}$ ,  $y_{min}$ ,  $y_{max}$ ,  $z_{min}$ ,  $z_{max}$ .

The output so far, when we run the Python script, will look something like this:

```
$ python screwpullout.py screwpullout.conf
   0.00 Reading configuration file screwpullout.conf
   0.00 Configuration:
        input file
                                      = sawbone.aim
        output file
                                      = sawbone.n88model
        bone material id
                                      = 127
        bone material Young's modulus = 6829.0
        bone material Poisson's ratio = 0.3
        screw material id
                                      = 90
        screw material Young's modulus = 69000.0
        screw material Poisson's ratio = 0.3
        screw displacement
                                      = 0.01
                                     = 4.5
        inner ring radius
        bone constraint max depth = 1.5
   0.00 Reading input data.
   0.07 Read 5775920 points from AIM file.
   0.07 Image bounds:
         11.9700 27.4740 11.7420 27.1320 0.1140 35.3400
```

## 7.8.5 Converting the image data to elements

As in the tutorial Compressing a cube revisited using vtkn88, we need to convert the input CT image data to a vtkUnstructured-Grid object representing the geometry. Again, we will use a vtkn88ImageToMesh filter for this purpose.

```
message("Converting to hexahedral cells.")
mesher = vtkn88.vtkn88ImageToMesh()
mesher.SetInputData(image)
mesher.Update()
mesh = mesher.GetOutput()
message("Generated %d hexahedrons" % mesh.GetNumberOfCells())
```

# 7.8.6 Defining material properties

Once again, we repeat the steps of the tutorial Compressing a cube revisited using vtkn88, and we generate a material table and two materials: bone and screw.

```
message ("Creating material table.")
material_table = vtkn88.vtkn88MaterialTable()
# Create an isotropic material for bone and add it to the table.
bone_material = vtkn88.vtkn88LinearIsotropicMaterial()
bone_material.SetName("bone")
bone_material.SetYoungsModulus(bone_material_modulus)
bone_material.SetPoissonsRatio(bone_material_poissons_ratio)
material_table.AddMaterial(bone_material_id, bone_material)
# Create an isotropic material for the screw and add it to the table.
screw_material = vtkn88.vtkn88LinearIsotropicMaterial()
screw_material.SetYoungsModulus(screw_material_modulus)
screw_material.SetPoissonsRatio(screw_material_poissons_ratio)
material_table.AddMaterial(screw_material_poissons_ratio)
```

## 7.8.7 Creating a vtkn88FiniteElementModel object

In the tutorial, Deflection of a cantilevered beam; adding custom boundary conditions and loads, we used vtkn88ApplyTestBase to combine the geometry with the model table into a vtkn88FiniteElementModel object. vtkn88ApplyTestBase didn't create any displacement boundary conditions or applied loads for us, but it did define some standard sets that we subsequently used to define our displacement boundary conditions and applied load. This time, those standard sets won't we very useful for us. So instead of vtkn88ApplyTestBase , we'll use an even more elementary model-creating filter called vtkn88FiniteElementModelGenerator , which creates a vtkn88FiniteElementModel object without any pre-defined sets.

### Tip

Actually, it is not quite true that we couldn't use need any standard sets. The standard set "face\_z1" would be the top surface of the screw, which is one of the sets that we need. However, for the purposes of demonstration, we'll show how to find that node set manually.

```
message("Constructing a finite element model object.")
generator = vtkn88.vtkn88FiniteElementModelGenerator()
generator.SetInputData(0, mesh)
generator.SetInputData(1, material_table)
generator.Update()
model = generator.GetOutput()
model.ComputeBounds()
bounds = model.GetBounds()
message("Model bounds:", (" %.4f"*6) % bounds)
```

Unlike vtkImageData objects, vtkUnstructuredGrid objects, from which vtkn88FiniteElementModel objects are derived, don't know their bounds unless you explicitly request them to be computed.

# 7.8.8 Writing an n88model file

Now that we have a vtkn88FiniteElementModel object, we can save it. Of course, the model isn't finished yet, but just as in the previous tutorial, we can still save it and examine it as we go.

```
message("Writing file %s" % n88model_file)
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInputData(model)
writer.SetFileName(n88model_file)
writer.Update()
```

# Important

Once again, in everything that follows it is intended that you add new lines to the script **before** the code (show just above) that saves the model to a file. Otherwise of course the saved n88model file won't reflect our additions and changes.

# 7.8.9 Adding history and log fields

By now you'll be familiar with adding History and Log fields to help us later trace back the details of the creation of this model. Let's add all this information (before the code to save the file!):

```
model.AppendHistory("Created by screwpullout.py version %s ." % script_version)
```

```
model.AppendLog(
"""screwpullout.py
Model of screw being pulled out of bone substitute material.
Using VTKN88 version %s .
Configuration file : %s
""" % (vtkn88.vtkn88Version.GetVTKN88Version(), config_file)
+ "\n".join(settings_text)) ①
```

• This looks a little bit complicated. "\n".join(settings\_text)) converts the Python list of strings to a single long string, inserting a line return ("\n") between each list item. We then just add it to the other string.

Now run the script. As a reminder, this is done with

```
$ python screwpullout.py screwpullout.conf
```

As shown in previous tutorials, we can retrieve the History and Log fields from the n88model file at any time with n88modelinfo:

```
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```

```
bone material id = 127
bone material Young's modulus = 6829.0
bone material Poisson's ratio = 0.3
screw material id = 90
screw material Young's modulus = 69000.0
screw material Poisson's ratio = 0.3
screw displacement = 0.01
inner ring radius = 4.5
bone constraint max depth = 1.5
```

## 7.8.10 Determining the screw orientation

In order to properly apply the desired constraints, we will need to know where the screw is. We can do this algorithmically, by calculating the principal axes of inertia of the screw using vtkn88TensorOfInertia . We are going to assume that the principal axis closest to the z axis is the screw axis. This won't be exactly true. Consider for example if the screw is cut off unevenly, then the principal axis of inertia won't be exactly the same as the screw axis, but for our purposes, it is good enough.

```
message("Determining screw geometry.")
moi = vtkn88.vtkn88TensorOfInertia()
moi.SetInputData(image)
moi.SetSpecificValue(screw_material_id) 1
moi.Update()
message("Number of cells belonging to screw: %d" % moi.GetCount())
message("Volume of screw: %.2f" % moi.GetVolume())
screwCenterOfMass = (moi.GetCenterOfMassX(),
                    moi.GetCenterOfMassY(),
                     moi.GetCenterOfMassZ())
message("Center of mass of screw: %.5f, %.5f, %.5f" % screwCenterOfMass)
screwAxis = moi.GetPrincipalAxisClosestToZ()
message("Axis of screw: %.5f, %.5f, %.5f" % screwAxis)
screwDistanceToBoundary = (bounds[5] - screwCenterOfMass[2]) / screwAxis[2]
screwCenterAtBoundary = (
    screwCenterOfMass[0] + screwDistanceToBoundary * screwAxis[0],
    screwCenterOfMass[1] + screwDistanceToBoundary * screwAxis[1],
    bounds[5]) 2
message("Distance from screw center of mass to top boundary: %.3f"  \leftrightarrow
   screwDistanceToBoundary)
message("Screw center at top boundary: %.3f, %.3f, %.3f" % screwCenterAtBoundary)
```

- This is how we limit the inertia tensor to be calculated only over the screw elements.
- 2 This is a simple geometric calculation: given the center of mass of the screw and the direction of the screw axis, find the intersection with the upper bound of the model.

Now we run it, and this part of the script generates output like this:

1.55 Determining screw geometry. 1.67 Number of cells belonging to screw: 449618 1.67 Volume of screw: 666.13 1.67 Center of mass of screw: 20.20622, 19.02016, 18.21310 1.67 Axis of screw: -0.00733, -0.00243, 0.99997 1.67 Distance from screw center of mass to boundary: 16.785 1.67 Screw center at boundary: 20.083, 18.979, 34.998

Comparing by eye with the rendering in ParaView, we can determine that these values are about right, so we give ourselves a gold star in advanced math and carry on.

# 7.8.11 Adding a boundary condition: applying a displacement to the screw end

We want to add a boundary condition to the screw where it intersects the boundary of the model. All these nodes lie on a plane, so they are easily found with the function AddNodesOnPlane provided in vtkn88NodeSetsByGeometry. Note that these nodes get associated with the FE model object, and we have to assign a name, in this case "screw\_top", so that we can refer later to this set.

```
message("Adding the screw_top boundary condition.")
vtkn88.vtkn88NodeSetsByGeometry.AddNodesOnPlane(
    2, ①
    bounds[5], ②
    "screw_top", ③
    model,
    screw_material_id) ④
message("Found %d nodes belonging to screw_top" %
    model.GetNodeSet("screw_top").GetNumberOfTuples()))
```

- The value 2 specified the z-axis (VTK and python being zero-indexed).
- 2 This is  $z_{max}$ .
- 3 The name of the node set we are creating.
- This argument is optional, and specifies that we only want nodes associated with material ID "screw\_material\_id". This is not actually necessary for the given data, since no elements of other material IDs intersect the  $z_{max}$  surface.

We want to be able to inspect this result, and ensure that we have in fact selected the nodes on the top of the screw. To do this, run the script to update the model file. Now, as in the tutorial Bending test of a radius bone with an uneven surface, we are going to use the tool n88extractsets to extract and visualize the node set.

```
$ n88extractsets sawbone.n88model
Reading N88 Model file : sawbone.n88model
Writing node set : sawbone_node_set_screw_top.vtp
```

The file sawbone\_node\_set\_screw\_top.vtp can be opened an visualized with ParaView. The nodes are shown in Figure 7.29, exactly on the end of the screw. This is what we want.



Figure 7.29: Screw top nodes, shown as white dots on the surface of the screw

### Tip

An alternative to using n88extractsets is to add lines to extract and save the node set directly to the script. We no longer recommend this, as it makes the script longer, more complex, and slower to run. However, for the record, this is how it would be done,

```
writer = vtk.vtkXMLUnstructuredGridWriter()
writer.SetInputData(model.DataSetFromNodeSet("screw_top"))
writer.SetFileName("screw_top_nodes.vtu")
writer.Update()
```

Having verified that we have found the set of nodes that we want, we can use the method ApplyBoundaryCondition of the vtkn88FiniteElementModel object to create a boundary condition. Note that we also give this the name "screw\_top\_-displacement".

```
model.ApplyBoundaryCondition(
    "screw_top", ①
    2, ②
    screw_displacement, ③
    "screw_top_displacement")
```

- The name of the set to which is apply the boundary condition.
- Once again the value 2 means the *z* direction
- 3 This variable is the numerical value of the displacement.

## 7.8.12 Fixing the nodes in a ring on the bone surface

This boundary condition is much more difficult, because we want to find nodes lying approximately in a ring on a rough surface. The approach we will take is to successively whittle down candidate nodes by applying a sequence of criteria, until we have finally just the nodes we want. These are the criteria:

- 1. Elements (cells) lie between a specified inner radius and outer radius, as measured from the screw axis.
- 2. Nodes lie within a maximum specified depth from the highest node satisfying the first criterion.
- 3. Nodes are visible from above.

### Tip

These selection criterion could in principle be applied in a different order. The reason for doing the selection by visibility last, is that it is computationally expensive, so we want to whittle down the candidate nodes/elements as much as possible before applying a visibility test.

### Step 1: Selecting cells within a hollow cylinder

VTK uses the concept of implicit functions which can be used to select points and cells within or without a certain geometry. Here we are going to use two vtkCylinder objects, and combine them with a difference operation with a vtkImplicitBoolean. This will result in a hollow cylinder. VTK has a filter object, vtkExtractGeometry, that will select points and cells based on a specified implicit function.

One complication is that set of Points in the output of vtkExtractGeometry are different than the original Points, and so the Point IDs will be different. However, we need to know the original Point IDs in order to be able to apply boundary conditions to the FE model. The solution to this is to use a concept in VTK called "Pedigree ID". These can be accessed with the method GetPedigreeIds from the PointData.

#### Note

Not every VTK data set will have Pedigree IDs. They must be added to the data set before we start chopping out subsets. However, by default vtkn88FiniteElementModelGenerator creates vtkn88FiniteElementModel objects with Pedigree IDs.

```
message ("Adding the fixed_bone_surface boundary condition.")
inner_cylinder = vtk.vtkCylinder() 1
inner_cylinder.SetRadius(inner_ring_radius)
inner_cylinder.SetCenter(screwCenterAtBoundary[0], 0, screwCenterAtBoundary[1]) 9
outer_cylinder = vtk.vtkCylinder()
outer_cylinder.SetRadius(outer_ring_radius)
outer_cylinder.SetCenter(screwCenterAtBoundary[0], 0, screwCenterAtBoundary[1]) 3
rotate_Y_to_Z = vtk.vtkTransform() 4
rotate_Y_to_Z.RotateX(90)
cylinder_difference = vtk.vtkImplicitBoolean()
cylinder_difference.AddFunction(outer_cylinder)
cylinder_difference.AddFunction(inner_cylinder)
cylinder_difference.SetOperationTypeToDifference()
cylinder_difference.SetTransform(rotate_Y_to_Z)
cylinder_extractor = vtk.vtkExtractGeometry()
cylinder_extractor.SetImplicitFunction(cylinder_difference)
cylinder_extractor.SetInputData(model)
cylinder_extractor.Update()
geometry_in_ring = cylinder_extractor.GetOutput() 
message("Found %d elements between inner and outer radii." % geometry_in_ring. ↔
   GetNumberOfCells())
```

- Important: vtkCylinder is by default oriented with a y axis of rotation. We will rotate to z axis of rotation later.
- **2**, **3** Note that the center is swapped  $y \leftrightarrow z$  because of the transform that will be applied.
- This is the transform we need to bring  $y \rightarrow z$ . Note that the transformation will be applied to input points, not to the cylinder geometry.
- The output will be another vtkUnstructuredGrid, which consists of a subset of the input geometry (including a subset of both Cells and Points).

Now, this is a good place to see what we have so far for a selection. There are two possibilites: we could write out geometry\_in\_ring with a vtkXMLUnstructuredGridWriter filter, or we could add the element IDs as a set to the model. Let's do the latter:

```
elements_in_ring = vtk.vtkIdTypeArray()  
elements_in_ring.DeepCopy(geometry_in_ring.GetCellData().GetPedigreeIds())
elements_in_ring.SetName("in_ring")
model.AddElementSet(elements_in_ring)
```

• To keep things clear, we're going to make a copy of the data array that is the PedigreeIds. This will allow us to modify it, by for example re-naming it, without affecting the original. There are two steps to this: creating a new empty vtkIdTypeArray and then using its DeepCopy method on the data array we want to copy.

Again, run the script to update the n88model file. We can now extract this element set from it as follows:

```
$ n88extractsets --element_sets sawbone.n88model
Reading N88 Model file : sawbone.n88model
Writing element set : sawbone_element_set_in_ring.vtp
```

Figure 7.30 shows this selection (*i.e.* the file sawbone\_element\_set\_in\_ring.vtp), together with the screw elements, shown for context. (We used a Threshold filter in ParaView to show just the screw cells from sawbone.n88model.) Figure 7.31 is another view of the same data. This view is more suited to inspecting the ring geometry of our selection. To construct this view, first hit the +z button on the toolbar in order to view exactly along the z axis. Then from View Settings under the Edit menu, select Use Parallel Projection. Finally, change the Representation of both data sets to Surface With Edges in order to show individual Cells.



Figure 7.30: Geometry as selected by hollow cylinder filter



Figure 7.31: Geometry as selected by hollow cylinder filter, seen in flat projection

### Step 2: Eliminating nodes below a certain depth

To select elements based on depth, as measured from the highest node in our set, we apply a similar approach as we did to select elements within the correct radii. We use a VTK implicit function, in this case a vtkBox, to specify the geometrical volume to which we want to limit our element set.

```
message("Filtering node set by depth.")
geometry_in_ring_bounds = geometry_in_ring.GetBounds() 0
message("Bounds of ring geometry: ", (" %.4f"*6) % geometry_in_ring_bounds)
box_bounds = (geometry_in_ring_bounds[0],
              geometry_in_ring_bounds[1],
              geometry_in_ring_bounds[2],
              geometry_in_ring_bounds[3],
              geometry_in_ring_bounds[5] - bone_constraint_max_depth,
              geometry_in_ring_bounds[5])
message("Limiting selection to box bounds: ", (" %.4f"*6) % box_bounds)
box = vtk.vtkBox()
box.SetBounds(box_bounds)
filter = vtk.vtkExtractGeometry()
filter.SetImplicitFunction(box)
filter.ExtractInsideOn()
filter.ExtractBoundaryCellsOn()
filter.SetInputData(geometry_in_ring)
filter.Update()
geometry_depth_filtered_ring = filter.GetOutput()
message("Found %d elements in bounding box." % geometry_depth_filtered_ring. \leftrightarrow
   GetNumberOfCells())
```

• Note that the *z<sub>max</sub>* bound of geometry\_in\_ring will be at the highest bit of bone in the ring.

Now just as before, we can create a corresponding element set for the purposes of inspection:

```
elements_depth_filtered_ring = vtk.vtkIdTypeArray()
elements_depth_filtered_ring.DeepCopy(geometry_depth_filtered_ring.GetCellData(). ↔
GetPedigreeIds())
elements_depth_filtered_ring.SetName("depth_filtered_ring")
model.AddElementSet(elements_depth_filtered_ring)
```

Run the script, and use n88extractsets to extract the element sets, and it will create a new file, sawbone\_element\_set\_depth\_filtered\_ring.vtp.

Figure 7.32 shows the remaining elements after filtering by depth.



Figure 7.32: Ring geometry after filtering by depth

## Step 3: Selecting only the nodes visible from above

We can use the function FindNodesOnVisibleSurface from vtkn88NodeSetsByGeometry for this purpose. We need to pass it a normal vector for the viewing direction, as well as an empty vtkIdTypeArray for storing the result.

```
message("Finding visible nodes.")
visibleNodesIds = vtk.vtkIdTypeArray() ①
normalVector = (0,0,1) ②
vtkn88.vtkn88NodeSetsByGeometry.FindNodesOnVisibleSurface(
   visibleNodesIds,
   geometry_depth_filtered_ring,
   normalVector,
   bone_material_id) ③
visibleNodesIds.SetName("ring_top_visible")
model.AddNodeSet(visibleNodesIds)
message("Found %d visible nodes." % visibleNodesIds.GetNumberOfTuples())
```

- This will store the result as a list of Point IDs.
- 2 This is the negative of the viewing direction.
- FindNodesOnVisibleSurface automatically returns the Pedigree Ids, provided that they exist on in input object (they do).

Again, run the script to update the n88model file. This time we want to extract the node sets

```
$ n88extractsets --node_sets sawbone.n88model
Reading N88 Model file : sawbone.n88model
Writing node set : sawbone_node_set_screw_top.vtp
Writing node set : sawbone_node_set_ring_top_visible.vtp
```

The resulting ring-shaped cloud of points (file sawbone\_node\_set\_ring\_top\_visible.vtp) is shown in Figure 7.33. These are the nodes to which we will apply our fixed boundary condition.



Figure 7.33: Bone nodes after filtering by visibility from above

### Defining the boundary condition on the bone

Now that we have a named node set for this constraint, it is easy to create the desired boundary condition, which we will name "fixed\_bone\_surface":

model.FixNodes("ring\_top\_visible", "fixed\_bone\_surface")

# 7.8.13 Specifying sets for post-processing

Just as we saw in the tutorial Deflection of a cantilevered beam; adding custom boundary conditions and loads, there remains one more step to complete the n88model file, and that is to identify the sets to be used for post-processing calculations by n88postfaim. We are interested in values calculated on the sets "ring\_top\_visible" and "screw\_top". However, when we have generated our own custom sets, as we have here, we must be careful about providing both node sets and the corresponding element sets to n88postfaim. If you review how we created the sets for generating boundary conditions, you will observe that we only generated the node sets. Fortunately, there is a method GetAssociatedElementsFromNodeSet of vtkn88FiniteElementModel that will identify the corresponding element set given a node set.

```
info = model.GetInformation()
pp_node_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_NODE_SETS()
pp_elem_sets_key = vtkn88.vtkn88SolverParameters.POST_PROCESSING_ELEMENT_SETS()
for setname in ["ring_top_visible", "screw_top"]:
    pp_node_sets_key.Append(info, setname)
```

```
elementSet = model.GetAssociatedElementsFromNodeSet(setname)
model.AddElementSet(elementSet)
pp_elem_sets_key.Append(info, setname)
```

After running the script, we can verify that these post-processing sets are in fact specified in the n88model file,

```
$ n88modelinfo --problems sawbone.n88model
Problems:
Name : Problem1
Part : Part1
Constraints : screw_top_displacement,fixed_bone_surface
PostProcessingNodeSets : ring_top_visible,screw_top
PostProcessingElementSets : ring_top_visible,screw_top
```

#### Tip

As before, it is possible to skip this step, and instead to specify the node and element sets to be used by n88postfaim on the command line of n88postfaim with the arguments

--node\_sets=ring\_top\_visible,screw\_top --element\_sets=ring\_top\_visible,screw\_top

We now have a complete n88model file. If you want, you can proceed to solve it using faim, as in previous tutorials. We leave it as an exercise to identify, from the analysis file, the net forces between the screw top and the constrained ring of bone.

This concludes the screw pull-out tutorial. In this tutorial we learned how to generate node sets based on complex criteria, to which we can then apply boundary conditions. This is the final tutorial in the series on learning vtkn88.

# 7.9 Additional examples

In addition to the tutorials, there are additional examples included in the examples directory. Currently these consist of

#### segment\_dicom

An example of reading a raw image file and performing a simple segmentation based on a density threshold and connectivity.

# **Chapter 8**

# **Special Topics**

# 8.1 Direct Mechanics

Microstructural organization plays an important role in macroscopic mechanical behaviour. For example, bone microarchitectural organization, as shown here in a human proximal femur, can exhibit patterns that are related to the macrostructural mechanical behaviour, and those patterns vary depending on the mechanical requirements at each location within the bone. A useful approach to characterizing the microstructural patterns (also referred to as "fabric") is to determine the anisotropic properties of subvolumes of bone. In some regions of the femur, for example, the bone microarchitecture will be highly aligned with the bone axis, but in other parts the alignment may be predominantly in a transverse orientation. The anisotropic properties typically need to be defined at several locations due to spatial variation.

Anisotropy can be defined in terms of either the fabric or mechanical behaviour. Methods for characterizing the fabric are based on techniques such as mean intercept length or star volume analysis, and a good resource is the paper by Odgaard (1997a). Essentially, fabric methods focus on the distribution of tissue microarchitecture. Alternatively, the mechanical elastic behaviour can be determined, and has been shown by Odgaard et al. (1997b) that the anisotropic fabric and mechanical properties are similar. This observation makes sense, and reinforces the concept that underlying bone micro-architecture is an important factor in determining mechanical behaviour. Here we focus on the determination of bone anisotropic elastic behaviour using a so-called *direct mechanics* assessment as proposed by van Rietbergen et al. (1996). In summary, six elastic finite element tests are performed on a cubic subvolume, and those results are used to define a  $6 \times 6$  stiffness matrix that relates stress to strain as per Hooke's Law,

$$\sigma = \mathbf{C}\varepsilon$$
 .

The most general anisotropic material requires 21 independent coefficients to fully characterize, but it is usually most convenient to assume there are planes of elastic symmetry, in which case there exists an orientation of a coordinate system where only 9 independent elastic coefficients are needed. See the section Linear Orthotropic Material. In this case,

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix}$$

Finite element models of real measurement data of biological materials do not exhibit perfect orthotropic symmetry, therefore the process of reducing the  $6 \times 6$  matrix from 21 independent coefficients to 9 involves finding an optimal coordinate system such that some of the coefficients are close to zero. It is reasonable to assume that bone mechanical behaviour can be reduced to a case of orthotropy; however, caution should be exercised as it is up to the user to determine whether this simplification is appropriate.

The basis of the direct mechanics approach is the application of six finite element tests to an appropriate bone subvolume:

- 1. uniaxial normal strain in the x-direction ( $\varepsilon_{xx}$ )
- 2. uniaxial normal strain in the y-direction ( $\varepsilon_{yy}$ )

- 3. uniaxial normal strain in the z-direction ( $\varepsilon_{zz}$ )
- 4. uniaxial shear strain in the x-direction  $(\gamma_{yz})$
- 5. uniaxial shear strain in the y-direction  $(\gamma_{zx})$
- 6. uniaxial shear strain in the z-direction  $(\gamma_{xy})$

These tests are applied under the conditions of unit engineering strain. Each test is evaluated for the six resulting stresses ( $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{xx}$ ,  $\sigma_{yz}$ ,  $\sigma_{zx}$ ,  $\sigma_{xy}$ ), thus providing directly the values of the 6×6 stiffness matrix. The stresses are calculated as a volume average, which can be shown to be equivalent to the surface stresses on the faces of the cube.

Finding the optimal rotation of the coordinate system to represent orthotropic behaviour involves first decomposing the stiffness matrix into symmetric and asymmetric components. The asymmetric component is discarded, as conservation laws require that the stiffness matrix be symmetric. (The asymmetric component thus consists entirely of measurement error.) An optimal rotation is then found that minimizes the coefficients that would be zero for a true orthotropic material expressed in the coordinate system of its planes of symmetry.

The primary outputs from the direct mechanics approach are the stiffness and compliance matrices ( $\mathbf{S} = \mathbf{C}^{-1}$ ) in the original coordinate system, as well as in the coordinate system of optimal orthotropy. The 3×3 rotation matrix **R** that describes the transformation from the specimen coordinate system to the optimal coordinate system is given; the rows are the principal axes in the original coordinate system. Finally, from the compliance matrix, the standard orthotropic elastic constants  $E_i$ ,  $v_{ij}$ ,  $G_{ii}$  are extracted. See Linear Orthotropic Material for the definitions.

The use of the n88directmechanics tool is described in detail in Section 9.5.

An example run of the *direct mechanics* analysis is shown below.

```
$ n88directmechanics test25a.aim
n88directmechanics version 6.0
Copyright (c) 2012, Numerics88 Solutions Ltd.
input_file
                             = test25a.aim
material_table
                            = homogeneous
                             = 6829.0
youngs_modulus
                             = 0.3
poissons_ratio
connectivity_filter
                             = on
    0.00 Reading image file test25a.aim
    0.00 Read 17576 points from image file.
    0.00 Applying connectivity filter.
    0.00 Masked out 0 unconnected voxels.
    0.00 Converting to hexahedral cells.
    0.01 Generated 7087 hexahedrons
    0.01 Creating material table.
    0.01 Creating three uniaxial models.
    0.03 Writing n88 model file: test25a_strain_xx.n88model
    0.14 Writing n88 model file: test25a_strain_yy.n88model
    0.25 Writing n88 model file: test25a_strain_zz.n88model
    0.34 Creating three symshear models.
    0.35 Writing n88 model file: test25a_strain_yz.n88model
    0.46 Writing n88 model file: test25a_strain_zx.n88model
    0.57 Writing n88 model file: test25a_strain_xy.n88model
    0.66 Calling solver on test25a_strain_xx.n88model
    2.20 Calling solver on test25a_strain_yy.n88model
    3.76 Calling solver on test25a_strain_zz.n88model
    5.23 Calling solver on test25a_strain_yz.n88model
    6.59 Calling solver on test25a_strain_zx.n88model
    7.87 Calling solver on test25a_strain_xy.n88model
    9.05 Reading n88 model file: test25a_strain_xx.n88model
    9.07 Reading n88 model file: test25a_strain_yy.n88model
    9.08 Reading n88 model file: test25a_strain_zz.n88model
    9.09 Reading n88 model file: test25a_strain_yz.n88model
```

```
9.10 Reading n88 model file: test25a_strain_zx.n88model
   9.11 Reading n88 model file: test25a_strain_xy.n88model
   Volume fraction = 0.45357
   Apparent stiffness matrix in specimen coordinate system
[[ 1571.653
           540.033 513.822
                               7.53 -121.22
                                                -57.959]
[ 540.033 2029.046 469.974
                              78.591 -53.69
                                                 -50.673]
513.822 469.974 1803.998
                                       -57.014
                              20.377
                                                -15.761]
                    20.377
[ 7.53
[ -121.22
            78.591
                              734.405
                                       -23.127
                                                 -36.557]
            -53.69
                     -57.014
                              -23.127 627.396
                                                 13.969]
                    -15.761 -36.557
 [ -57.959
           -50.673
                                      13.969
                                                 745.749]]
   Apparent compliance matrix in specimen coordinate system
[[ 7.570e-04 -1.586e-04 -1.704e-04 1.977e-05 1.170e-04
                                                         4.323e-051
[ -1.586e-04
             5.610e-04 -1.000e-04 -5.441e-05 5.808e-06 2.090e-05]
 [-1.704e-04 -1.000e-04 6.294e-04 -4.883e-06 1.569e-05 -7.273e-06]
[ 1.977e-05 -5.441e-05 -4.883e-06 1.372e-03 4.787e-05 6.410e-05]
 [ 1.170e-04 5.808e-06 1.569e-05 4.787e-05 1.621e-03 -1.819e-05]
 [ 4.323e-05 2.090e-05 -7.273e-06 6.410e-05 -1.819e-05 1.349e-03]]
   Material parameters in specimen coordinate system
   Exx = 1320.98
   Eyy = 1782.54
   Ezz = 1588.79
   Gyz = 728.81
   Gzx = 617.06
   Gxy = 741.27
       ____
   nu_y = 0.28270
   nu_zx = 0.27081
nu_xy = 0.20950
   nu_zy = 0.15888
   nu_xz = 0.22516
   nu_yz = 0.17825
   _____
                            _____
   Optimum rotation matrix R:
[[ 0.32957 -0.83991 -0.4312 ]
[ 0.30346 0.52671 -0.79403]
[ 0.89404 0.13084 0.42846]]
   Apparent stiffness matrix in best orthotropic coordinate system
[[ 2197.117
           466.121 496.104 30.725 39.277
                                                 6.441]
[ 466.121 1852.499 506.856 32.259 14.028
                                                 -0.103]
                                      -28.362
[ 496.104 506.856 1464.576
                               -5.755
                                                 14.264]
           32.259 -5.755 650.075
[ 30.725
                                      -35.665
                                                -15.051]
[ 39.277
                                      697.661
             14.028
                     -28.362
                              -35.665
                                                 8.234]
 [ 6.441
             -0.103 14.264
                              -15.051
                                      8.234
                                                 705.066]]
   Apparent compliance matrix in best orthotropic coordinate system
[[ 5.068e-04 -8.804e-05 -1.419e-04 -2.273e-05 -3.367e-05 -1.863e-06]
[ -8.804e-05 6.126e-04 -1.826e-04 -2.865e-05 -1.630e-05 4.167e-06]
[ -1.419e-04 -1.826e-04 7.952e-04 2.496e-05 4.544e-05 -1.482e-05]
[ -2.273e-05 -2.865e-05 2.496e-05 1.546e-03 8.154e-05 3.175e-05]
[ -3.367e-05 -1.630e-05 4.544e-05 8.154e-05 1.442e-03 -1.571e-05]
```

[-1.863e-06 4.167e-06 -1.482e-05 3.175e-05 -1.571e-05 1.419e-03]] Material parameters in best orthotropic coordinate system Exx = 1973.20Eyy = 1632.50Ezz = 1257.55646.74 Gyz = 693.58  $G_{Z,X} =$ Gxy = 704.48  $nu_yx = 0.14372$ 0.17848 nu\_zx = 0.17371 nu\_xy = 0.22968 nu\_zy =  $nu_xz = 0.28004$ nu\_yz = 0.29816

9.47 Done.

# 8.2 Pistoia Failure Load Estimate

The failure load for a linear elastic model is based on the work by Dr. Walter Pistoia (Pistoia 2001a and 2001b). Numerics88 provides a tool, n88pistoia that can be used to carry out these calculations. In general, it is more accurate and preferable to solve an elastoplastic model in order to obtain failure loads. However, we include the Pistoia tool, mostly for those who wish to compare current data to older results on which a Pistoia analysis was done.

The basic principal is that failure load is defined as the load at which a pre-defined volume of tissue (percentage critical volume) exceeds a pre-defined Energy Equivalent Strain (critical EES). Typical values are 2.0% and 0.007, respectively. It should be noted that the so-called Pistoia criterion is not a standard failure criteria used in classical mechanics of materials; however, it has been extensively validated with experimental testing of cadaver bones, and it is the most widely used and accepted criterion for image-based linear FE modelling.

The *first* sub-table contains the failure load information (the sub-table is denoted by a series of horizontal dots). The calculation of the failure load requires post-processing the EES for each element of the solved linear FE model. After ordering the EES in a histogram, the actual strain at the critical volume threshold (e.g., 2%) is determined and reported in the table as EES at vol\_crit. As this is a linear FE model, a scale-factor for this EES can be determined relative to the critical EES, and this is captured in a defined factor. A table of factors is provided at the bottom of the Pistoia Failure Load Estimate table, and the factor associated with the defined critical volume and critical EES is reported specifically in this first sub-table (other values of critical volume and critical EES could be applied if necessary using the alternative table factors). Knowing the total reaction force of the solved model (usually RFz) and the actual EES value at the critical volume, a linear factor can be applied to estimate the failure load =RFz × factor.

#### Note

Although a similar process can be applied to determine the torsional failure load (and is reported as torsional failure load) there have not been any experimental validations of this technique published to date. It is not recommended to use the reported torsional failure load until experimental validation is completed. Nevertheless, it is provided here for the users' convenience.

The *second* sub-table contains a summary of the axial and torsional stiffness values, and these are identical to the previous corresponding tables. For example, RFz from node set 1 has already been reported in Nodel Forces as total  $F_z$ . They are reported again in this table for convenience.



### Important

All failure loads are calculated assuming that axial compression or torsion was applied along the *z*-axis in the Data Frame.

The *third* sub-table contains a summary of the histogram results for the analysis of EES. All materials defined in the model are pooled for this histogram (i.e., cortical bone and trabecular bone), and it is the basis for determining the EES at the critical volume used for the failure load calculation. It is important to note that the user has the option to pre-define a material that is to be excluded from the failure load analysis, and that excluded material is reported at the top of the table (Excluded material id). This is useful, for example, if the FE model contains platens that should not be included in the failure load analysis (i.e., the failure load of the platens are not of interest).

The *fourth* sub-table contains a summary of the number of elements that exceed critical EES, and is broken down by material definition. This information allows the user to determine, for example, whether failure was based on cortical bone versus trabecular bone.

The *fifth* sub-table contains factors that could be used (by user hand calculation) to determine the estimated failure load for different critical volumes or critical EES.

Table 1: Pistoia Failure Load Estimate \_\_\_\_\_ Pistoia Criterion for Energy-Equivalent-Strain (EES) (\*) Results valid for linear, isotropic model only. (\*) Warning: Torsion failure load not validated. Caution! Number of elements in analysis: 349829 Excluded material id: none Critical volume (%): 2.0000 Critical EES: 0.0070 EES at vol crit: 0.0131 Factor (from table): 0.5332E+00 Failure load (RFz \* factor) [N]: -0.3248E+04 🛈 Torsional failure load (Tz \* factor) [Nmm]: 0.9764E-03 Axial and Torsional Stiffness: -0.6091E+04 RFz (node set 1) [N]: Uz (node set 1) [mm]: -0.9020E-01 Axial stiffness [N/mm]: 0.6753E+05 2 Tz (node set 1) [Nmm]: 0.1831E-02 Rotz (node set 1) [rad]: -0.1787E-03 Torsional stiffness [Nmm/rad]: -0.1025E+02 3 \_\_\_\_\_ Distribution of energy-equivalent-strain: EES = sqrt(2U/E). EES average 0.6135E-02 std\_dev 0.3210E-02 minimum 0.1332E-07 maximum 0.3725E-01 skewness 0.4787E+00 kurtosis 0.9386E+00 median 0.6089E-02 Distribution of failed materials. material # els 8 1454 5543 127 20.7803 100 79.2197 🛛

	total	6997	100.0000			
Factor t	able:					
	crit_vol	crit_ees				
90	# vox	0.0050	0.0060	0.0070	0.0080	0.0090
1.00	349829	0.3400E+00	0.4080E+00	0.4759E+00	0.5439E+00	0.6119E+00
2.00	699658	0.3809E+00	0.4570E+00	0.5332E+00	0.6094E+00	0.6855E+00
3.00	1049487	0.4071E+00	0.4886E+00	0.5700E+00	0.6514E+00	0.7329E+00
4.00	1399316	0.4274E+00	0.5129E+00	0.5984E+00	0.6838E+00	0.7693E+00
5.00	1749145	0.4444E+00	0.5333E+00	0.6222E+00	0.7111E+00	0.8000E+00
6.00	2098974	0.4582E+00	0.5498E+00	0.6414E+00	0.7331E+00	0.8247E+00
7.00	2448803	0.4703E+00	0.5644E+00	0.6585E+00	0.7525E+00	0.8466E+00

- Estimated failure load of the bone in uniaxial compression, given the critical volume of 2% and critical EES of 0.0070.
- Calculated based on the total Fz (also termed RFz) of node set 1 divided by the average displacement Uz of the surface defined by node set 1.
- Calculated based on the total Tz of node set 1 divided by the average displacement Uz of the surface defined by node set 1.
- Indicates that approximately 79% of the failed voxels comprising the 2% critical volume were in the trabecular tissue, while only 21% were in the cortical tissue.

# **Chapter 9**

# **Command Reference**

## Table 9.1: List of Faim command-line programs

Module	Description
faim	Convenience utility that calls n88solver, n88derivedfields and n88postfaim in
	sequence.
n88copymodel	Copy, convert or compress a finite element model file.
n88compress	Compress a finite element model file in-place.
n88derivedfields	Calculate additional field values (forces, stress, strain, etc) that are not generated by
	n88solver.
n88directmechanics	Perform <i>direct mechanics</i> calculations.
88evaluate	Calculate some values that indicate the correctness of the solution.
n88extractfields	Extracts specified solution fields as tabular text data.
n88extractsets	Extract node sets, element sets and constraint sets and write them to VTK PolyData
	(.vtp) files.
n88modelgenerator	Generate a finite element model from a segmented 3D image.
n88modelinfo	Print summary information for a Numerics88 FE model file.
n88pistoia	Estimate failure loads from a linear model.
n88postfaim	Generate tables of standard post-processing quantities.
n88solver (_sl and _sp)	Solvers suitable for small-strain models with linear elastic material definitions (_el)
	or with non-linear elastoplastic material definitions (_ep).
n88tabulate	Tabulate values from n88postfaim output files for importing into a spreadsheet.

# 9.1 faim

A convenience utility that calls n88solver, n88derivedfields and n88postfaim in sequence on the specified model file.

The analysis file produced by n88postfaim will be named after the input file, with "\_analysis.txt" replacing the extension of the input file.

### Note

Although the underlying work is performed by different programs, the faim utility produces the same results as did running faim in version 5.x. For those accustomed to previous faim versions, this utility provides a work-flow that is unchanged.

The command line arguments of faim are listed below. As they are passed through to the programs doing the work, they are grouped by program that they are passed to. In each case the options are identical to those of the program doing the work.

### Arguments passed to n88solver

convergence\_tolerance
device
engine
license\_check
maximum\_iterations
quiet
restart
threads
threshold\_window

For details, refer to n88solver.

### Arguments passed to n88derivedfields

device engine quiet threads

For details, refer to n88derivedfields.

## Arguments passed to n88postfaim

element\_sets
node\_sets
quiet
rotation\_center

For details, refer to n88postfaim.

# 9.2 n88copymodel

## Description

Copy, convert or compress a finite element model file.

### Usage

```
n88copymodel [-h] [--compress] input [input2] output
```

File formats are automatically identified by their extensions. Ambiguous input file extensions are resolved by examining the file.

Two input files are allowed if the first is a FAIM version 5 input file (.inp), and the second is a FAIM version 5 output file (.dat). This will create a complete, solved n88model file. Either .inp or .dat can also be converted individually, but in the case of .dat files, the resulting n88model file will be incomplete, as the .dat file alone does not contain either material definitions or constraints; however, it can be rendered and processed by n88postfaim, but not re-solved.

## SUPPORTED INPUT FORMATS

- Numerics88 model file (.n88model)
- Abaqus input file (.inp)
- Faim version 5 input file (.inp)
- Faim version 5 output file (.dat)

SUPPORTED OUTPUT FORMATS

- Numerics88 model file (.n88model)
- Abaqus input file (.inp)
- VTK XML Unstructured Grid file (.vtu)

## Tip

VTK XML Unstructured Grid files can be read be and rendered by ParaView, even without the Numerics88 plugins. They include the complete geometry, plus any solution fields, but lack any constraint or material information.

### Table 9.2: n88copymodel optional arguments

Option	Description
-h,help	Show help and exit.
compress, -c	Use compression when writing the output file if the file format supports it.
	Compressed n88model files do not need to be uncompressed in order to use them:
	they can be used in all cases exactly like uncompressed files. Compressed files may
	be slower to read, and are particularly slower to write.

### Note

If you compress an n88model file, and then run either n88solver or n88derivedfields on it, it will end up in a mixed state, where the original data is compressed, but the new data added by n88solver or n88derivedfields is uncompressed. There is nothing wrong with this as the file is still completely valid and useable. However, usually if compression is important, one wants the entire file data compressed. Therefore, we recommend not compressing the file until you have completed all the normal processing steps on it. It is of course possible to convert a partially compressed n88model file to a fully compressed n88model file by running n88copymodel or n88compress on it again.

See also the section Converting Faim version 5 file formats.

# 9.3 n88compress

n88compress FILENAME

is an alias for

n88copymodel --compress FILENAME FILENAME

Refer to the documentation for n88copymodel.

# 9.4 n88derivedfields

### Description

Calculates additional field values (forces, stress, strain, etc) that are not generated by n88solver.

For discussion of use, see the section on using n88derivedfields in the Post-processing chapter.

## Usage

n88derivedfields [options] input\_file

### Arguments

Argument	Description
help [-h]	Print help and exit.
engine [-g] arg (=mt)	Set the engine. Valid values are mt for the multi-threaded CPU engine and nv for the
	nVidia GPU engine. Note that a license is required to use the GPU engine.
threads [-t] arg (=0)	Set the number of threads for the mt engine (0=automatic). Automatic will select one
	thread per physical processing core on the system, or one thread per 2048 elements,
	whichever is less.
device [-d] arg (=0)	Set the nVidia CUDA device to use. Multiple devices may be specified in a comma
	delimited list.
quiet [-q]	Suppress output to terminal (except for error messages).
precision arg (=single)	Set the floating point precision used. Values: single, mixed, double.

Table 9.3:	n88derivedfields	arguments
------------	------------------	-----------

# 9.5 n88directmechanics

# Description

Perform direct mechanics calculations. See Section 8.1 in the Special Topics chapter.

## Usage

```
n88directmechanics [-h] [-c FILE] [--generate] [--solve] [--analyze]
[--material_table {homogeneous,homminga}]
[--youngs_modulus YOUNGS_MODULUS]
[--poissons_ratio POISSONS_RATIO]
[--orthotropic_parameters ORTHOTROPIC_PARAMETERS]
[--homminga_maximum_material_id HOMMINGA_MAXIMUM_MATERIAL_ID]
[--homminga_modulus_exponent HOMMINGA_MODULUS_EXPONENT]
[--connectivity_filter {on,off}]
input_file
```

Table 9.4: n88directmechanics input arguments

Option	Description
input_file	An image file with segmented data. Note that the file name of the original image file
	should be used even when the only action issolve and/oranalyze; the
	n88model file names will be derived from the image file name. Supported input
	formats:
	- DICOM (a directory)
	- Scanco AIM (.aim)
	- MetaImage (.mha or .mhd)
	- VTK XML ImageData (.vti)

### Table 9.5: n88directmechanics action arguments

Option	Description
generate	Generate models. (Generates 6 n88model files.)
solve	Solve models. (n88model files are updated with solutions.)
analyze	Perform direct mechanics analysis on solved files.

Multiple action arguments may be specified. If no action argument is specified, it is equivalent to specifying them all.

### n88directmechanics material specification arguments

```
material_table
youngs_modulus
poissons_ratio
orthotropic_parameters
homminga_maximum_material_id
homminga_modulus_exponent
```

These arguments are identical to the equivalent arguments of n88modelgenerator. See Material specification parameters.

## Table 9.6: n88directmechanics optional arguments

Option	Description
-h,help	Show help and exit.
-c FILE,config FILE	Specify a configuration file. The configuration file may specify any arguments that
	take a value, one per line, in the format name=value (leave the double dash "" off of
	the argument name). This format is identical to n88modelgenerator. See Section 2.1.

### n88directmechanics additional parameters

connectivity\_filter
spacing

These arguments are identical to the equivalent arguments of n88modelgenerator. See Additional parameters.

# Тір

There are no options passed to the solver. If this is required, run n88directmechanics with the --generate action, then manually run n88solver on each of the resulting n88model files, using the desired solver options, then run n88direc tmechanics again with the --analyze action.

# 9.6 n88evaluate

### Description

A tool to evaluate the quality of solutions.

For discussion of use, see the section on using evaluating solution quality and the section section on using evaluating nonlinear solution quality.

### Usage

n88evaluate [options] input\_file

# Arguments

Table 9.7: n88evaluate arguments

Argument	Description
help [-h]	Print help and exit.
sparse [-s]	Use sparse matrices for calculation. This is the default, but requires that scipy be installed.
dense [-t]	Use dense matrices for calculation. This does not require scipy to be installed, but as the memory requirements scale as the square of the number of degrees of freedom in the problem, this is feasible only for very small problems.

# 9.7 n88extractfields

# Description

Extracts specified solution fields as tabular text data.

# Usage

n88extractfields [-h] [--output\_file OUTPUT\_FILE] fields input\_file

Table 9.8: n88extractfields positional arguments

Option	Description		
fields	A comma-delimited list of names of solution fields to extract. May be the name of		
	either a solution node value (e.g. "Displacement") or a solution element value (e.g.		
	"Stress"; see also Calculating additional solution fields with n88derivedfields)		
	Additionally, "NodeNumber", "ElementNumber", "MaterialID",		
	"NodeCoordinates", "ElementCoordinates" or "Topology" can be specified. Element		
	coordinates are the centers of the elements. Topology gives for each element the 8		
	node numbers of the nodes constituting the element. The order is as in the		
	n88model file, refer to the file specification. All fields must be the same length,		
	which practically means that they must either be all node values or all element values.		
input	The model file.		

Table 9.9: n88extractfields optional arguments

Option	Description
-h,help	Show help and exit.
output_file OUTPUT_FILE, -o	Output file. If not specified, output will go to STDOUT.
OUTPUT_FILE	

## Examples

This will extract the displacement values as an  $N \times 3$  array, where N is the number of nodes:

```
$ n88extractfields Displacement mymodel.n88model
                -0.00136573
-0.00136573
                                 0.0
-0.000770869
                -0.00142601
                                0.0
-0.000218384
                -0.00141035
                                 0.0
0.000218384
                -0.00141035
                                 0.0
0.000770869
                -0.00142601
                                 0.0
0.00136573
                -0.00136573
                                 0.0
-0.00142601
                -0.000770869
                                 0.0
. . .
```

This example will extract both element number and corresponding stress. As the stress is 6-valued, this makes a total of 7 values per row of output:

\$	n88extractfields	ElementNumber,Stress	mymodel.n88model	1		
1	-0.752387	-0.752387	-69.0185	0.965844	0.965844	$\leftrightarrow$
	-0.00933552					
2	-4.98979	-1.50565	-73.2319	0.629349	0.690826	$\leftrightarrow$
	1.61737					
3	-6.35569	-0.494144	-74.5778	0.486541	-4.27155e-16	$\leftrightarrow$
	-5.6954e-16					
4	-4.98979	-1.50565	-73.2319	0.629349	-0.690826	$\leftrightarrow$
	-1.61737					
5	-0.752385	-0.752386	-69.0185	0.965844	-0.965844	$\leftrightarrow$
	0.00933552					
6	-1.50565	-4.98979	-73.2319	0.690826	0.629349	$\leftrightarrow$
	1.61737					
7	-1.50565	-4.98979	-73.2319	0.690826	-0.62934	
• •	•					

# 9.8 n88extractsets

## Description

Extract node sets, element sets and constraint sets and write them to VTK PolyData (.vtp) files which can be opened with ParaView. This is mostly useful for visualizing sets, boundary conditions and applied forces. For nodes sets and constraints, these files will consist of a collection of vertices.

### Usage

n88extractsets [-h] [--constraints] [--node\_sets] [--element\_sets] input

Table 9.10:	n88extractsets	arguments
-------------	----------------	-----------

Option	Description
-h,help	show this help message and exit
constraints, -C	Extract constraints.
node_sets, -N	Extract node sets.
element_sets, -E	Extract element sets.
If no arguments are specified, all types of sets will be extracted.



#### Warning

This utility will generate file names based on the names of the sets, and will overwrite existing files with the same names without warning.

## 9.9 n88modelgenerator

#### Description

Generates a finite element model from a segmented 3D image.

Refer to the chapter on using n88modelgenerator.

#### Usage

n88modelgenerator [options] input\_file [output\_file]

#### Supported input image file formats

n88modelgenerator currently supports the following input formats:

- DICOM (automatically selected when a directory is given as the input),
- Scanco .aim files,
- ITK MetaImage files (.mha) or (.mhd),
- VTK XML Image Data files (.vti),
- existing Numerics88 Model file (.n88model)

#### Note

There are some limitations when reading DICOM files. In particular, encapsulated format cannot be read. It is sometimes not possible to determine the *z*-spacing from DICOM files. In this case use the option spacing.

#### Note

If an n88model file is provided as an input file, the mesh (i.e. the points and elements) will be taken from the input, as well as any possible solution fields. A new material table and new constraints will be generated. This is useful for incremental loading tests of nonlinear models, as it allows the boundary conditions to be updated while preserving an existing solution.

#### Supported output file formats

The standard output format of n88modelgenerator is an n88model file (see Appendix C). If you specify an output file with extension .n88model, the n88model file format will be used. This is the default output type, and if no output file is specified, an output file will be generated from the stem of the input file, with the extension .n88model appended.

n88modelgenerator also supports the output of Abaqus input files. An Abaqus input file will be generated whenever an output file with extension . inp is specified.

#### Input and output parameters

Input and output parameters specify the files that are used for input and output.

Argument	Description
input_file	Specify the name of the input file. Note that it is not necessary to explicitly use
	"input_file" on the command line, as the first positional argument (i.e. the first
	argument not starting with a dash), is taken to be the input file.
output_file	Specify the name of the output file. If not specified, a default output file name will be
	used, which is of the form [input]_[test_type].n88model. Note that it is
	not necessary to explicitly use "output_file" on the command line even if you want
	to specify the output file name, as the second positional argument, (i.e. the second
	argument not starting with a dash), if present, is taken to be the output file. However
	the type of output file is determined by the extension of output_file, therefore if
	output different than the default type (n88model) is desired, the output file must be
	explicitly specified.

#### Table 9.11: n88modelgenerator Input and Output Parameters

### **Test configuration parameters**

Test configuration parameters define the mechanical test that will be applied to the object in the image.

Argument	Description
test	Specify test type. Valid values are uniaxial, axial, confined, bending,
	torsion, symshear and dshear. See Standard Tests.
test_axis	Specify the test axis. See Test Orientation. Valid values are <i>x</i> , <i>y</i> , and <i>z</i> . The default is <i>z</i> .
normal_strain	For a compression type test, specifies an apparent level strain. Negative values correspond to compression. Strain is the default if neither strain nor displacement are specified. Default -0.01, corresponding to 1% compressive strain.
shear_strain	For a symshear test, this sets the apparent engineering shear strain applied to the model. Unitless. Default 0.01.
strain	Shortened equivalent of either normal_strain or shear_strain, depending on the test type.
displacement	Specify an applied displacement (with units of length) for a compression type test. Negative values correspond to compression. This parameter is exclusive with normal_strain: one or the other may be used, but not both.
pin	Fully define the constraints for a uniaxial model by adding an arbitrary pinned point to prevent lateral translation, and a second partially pinned point to prevent lateral rotation. If this option is off, the system of equations for a uniaxial test is singular. Faim can solve it regardless, and will in fact typically solve it faster. This option is ignored for test types other than uniaxial. Valid values are off, center, corner and on. The value corner adds a pin at the element with the minimum $z,y,x$ coordinates in the Test Frame ( <i>i.e.</i> select by minimum $z$ , then by minimum $y$ , then by minimum $x$ ). center adds a pin at the element closest to the center $x,y$ position in the Test Frame. (The $z$ coordinate is not considered, unless two elements are equally close to the $x,y$ center, in which case the one with smallest $z$ is selected.) The value on is equivalent to center. Default is off.

#### Table 9.12: (continued)

Argument	Description
central_axis	The $x, y$ coordinates (in the Test Frame) of the central axis, which is parallel to the $z$
	axis (in the Test Frame). Example: 0, 0. Alternatively, you can specify
	center_of_mass or center_of_bounds. The default is
	center_of_mass. The central axis is used in bending and torsion tests.
bending_angle	The degree of tilt between the top and bottom surfaces in a bending test. Units are
	degrees. The default is 1°.
neutral_axis_angle	The angle of the neutral axis in the $x, y$ plane (in the Test Frame) in a bending test. 0°
	is parallel to the x-axis. Units are degrees. Default is 90°, parallel to the y-axis.
shear_vector	The amount of shear displacement of the top surface as a vector in the <i>x</i> , <i>y</i> plane (in
	the Test Frame) for a dshear test. Units are length units if scale_shear_to_height is
	off, otherwise a unitless ratio. Default is 0.01,0.
scale_shear_to_height	If on, shear_vector will be scaled by the height of the model extent (in the $z$ direction
	in the Test Frame) to determine the shear displacement applied for a dshear test.
	Valid values are on and off. Default is on.
twist_angle	Amount of rotation of the top surface in a torsion test. Units are degrees. Default is
	1°.

#### Surface detection parameters

Surface detection parameters modify how the top and bottom surfaces of the object image are identified. For most test types, the principle boundary conditions are applied to these two surfaces. If not specified, by default these surfaces are identified as all nodes (or elements) at the top or bottom extent of the input.

Argument	Description
top_surface	Specify method of selecting top surface. Valid values are intersection and visible. See Uneven surfaces.
bottom_surface	Specify method of selecting bottom surface. Valid values are intersection and visible. See Uneven surfaces.
top_surface_maximum_depth	Specify the maximum depth for identifying the top surface. Only applies if top_surface = visible. If zero, depth is unlimited. Depth is measured from the top boundary of the volume. Default is zero.
bottom_surface_maximum depth	Specify the maximum depth for identifying the bottom surface. Only applies if bottom_surface = visible. If zero, depth is unlimited. Depth is measured (upwards) from the bottom boundary of the volume. Default is zero.
top_constraint_material_id	Apply boundary conditions at the top surface only to cells and nodes of the specified material ID.
bottom_constraint_material_id	Apply boundary conditions at the bottom surface only to cells and nodes of the specified material ID.

Table 9.13: n88modelgenerator Surface Detection Parameters

### Material specification parameters

Material specification parameters are used to specify material definitions, and to select a material table that maps material IDs to material definitions.

Argument	Description
poissons_ratio	Specify isotropic Poisson's ratio. The default is 0.3.
youngs_modulus	Specify isotropic Young's modulus. The default is 6829.
orthotropic_parameters	Specify orthotropic parameters as $E_x, E_y, E_z, v_{yz}, v_{zx}, v_{xy}, G_{yz}, G_{zx}, G_{xy}$ . If not set, isotropic parameters will be assumed. <b>Important</b> : There are two common conventions for ordering the mixed index quantities $v_{ij}$ and $G_{ij}$ . Numerics88 software uses the ordering <i>YZ</i> , <i>ZX</i> , <i>XY</i> . It is important to observe this when specifying orthotropic properties in n88modelgenerator, as these are input in the form of an ordered list.
plasticity	Specify an elastoplastic yield criterion. Specify as several values separated by commas. The first value is an elastoplastic yield criterion name; subsequent values are numeric arguments appropriate to the method. Supported methods: VonMises, Y: Y is the yield strength. Refer to von Mises yield criterion. MohrCoulomb, YT, YC: YT is the yield strength in tension and YC is the yield strength in compression. Refer to Mohr-Coulomb yield criterion.
material_table	Specify method for generating material table. Valid values are homogeneous and homminga. homogeneous assigns the same material to all material IDs. homminga generates a table of materials according to Homminga et al. Refer to Homminga material table for details.
homminga_maximum_material id	Specify the maximum material ID used in Homminga density to modulus conversion. The default is 127.
homminga_modulus_exponent	Specify exponent used in Homminga density to modulus conversion. The default is 1.7.

## Additional parameters

Argument	Description
spacing	Force the spacing of the input image. This is sometimes required for DICOM files,
	for which the z-spacing sometimes cannot be determined. Values should be given as
	a comma-delimited list of $x, y, z$ values. $e.g. 0.5, 0.5, 0.5$ .
connectivity_filter	Enable/disable connectivity filtering which extracts only the largest connected object
	in the input image. See Ensuring connectivity in the chapter about vtkn88 for a
	discussion of this issue. Valid values are on, off and warn. The default is on.

Table 9.15: n88modelgenerator Additional Parameters

#### Solver parameters

Solver parameters affect the execution of the solver. They are independent of the model creation, and are specific to the solver used. If given as arguments to n88modelgenerator, they will be stored in the n88model file. However for most purposes, it is better to leave these out of the n88model file and either use the defaults as selected by the solver, or else to specify them as command line arguments directly to the solver. See n88solver.

Argument	Description
convergence_tolerance	Specify convergence tolerance for conjugate gradient iterations. If not specified a
	default value will be used. See Generating the displacements with n88solver.
maximum_iterations	Specify the maximum number of conjugate gradient iterations. If not specified a default value will be used. The default is 30000. See Generating the displacements with n88solver.
plastic_convergence_tolerance	Specify convergence tolerance for plastic iterations. If not specified a default value will be used.
maximum_plastic_iterations	Specify the maximum number of plastic iterations. If not specified a default value
	will be used. The default is 100.

#### Table 9.16: n88modelgenerator Solver Parameters

## 9.10 n88modelinfo

#### Description

Print summary information for a Numerics88 finite element model file.

Usage

```
n88modelinfo [-h] [--active] [--history] [--log] [--materials]
        [--parts] [--node_sets] [--element_sets] [--sets]
        [--constraints] [--problems] [--solutions]
        input_file
```

Table 9.17: n88modelinfo positional arguments

Option	Description
input_file	The .n88model file to read.

Table 9.18: n88modelinfo action arguments:

Option	Description
active	List active solution, problem and part.
history	Show history.
log	Show log.

#### Table 9.18: (continued)

Option	Description
materials	List defined materials.
parts	Show parts.
node_sets	Show nodesets.
element_sets	Show elementsets.
sets	Show both node and element sets. (Equivalent tonode_sets andelement_sets.)
constraints	Show constraints.
problems	Show problems.
solutions	Show solutions.

Multiple action arguments may be specified. If no action argument is specified, it is equivalent to specifying them all.

Table 9.19: n88modelinfo optional arguments

Option	Description
-h,help	Show help and exit.

## 9.11 n88pistoia

#### Description

Calculate Pisotia yield critera. This is a method if estimating yield strength from linear solutions. In general, it would be preferable to use a non-linear elastoplastic model to calculate yield strengths. This utility is provided mostly for comparing with older results.

For discussion of use, see the section on the Pistoia failure load estimate in the special topics chapter.

Note that n88pistoia is implemented in python (in tools/pistoia.py), so you can copy it and modify it should you wish to modify the analysis.

#### Usage

```
n88pistoia [options] input_file
```

#### Arguments

Argument	Description
help [-h]	Print help and exit.
output_file [-o] arg	Specify an output file. If no output file is specified, output will go to STDOUT.
constraint [-n] arg	Specify the constraint (i.e. boundary condition or applied load) to use for analysis.
	This is the surface to which forces are applied. The default ("top_displacement") will
	work for models generated with n88modelgenerator.
rotation_center [-c] arg	Specify the spatial center used for calculation of angular quantities. The argument
	must be given as a triplet of coordinates. If not specified, the value will be read from
	the input file. If not available, no angular quantities will be calculated.
include [-i] arg	Only elements with the specified material IDs will be included in the calculation.
	Multiple IDs can be specified in a comma-delimited list (e.g. 100,101,105).

#### Table 9.20: n88pistoia arguments

#### Table 9.20: (continued)

Argument	Description
exclude [-e] arg	All elements with the specified material IDs will be excluded from the calculation.
	Multiple IDs can be specified in a comma-delimited list (e.g. 100,101,105).
quiet [-q]	Suppress output to terminal (except for error messages).

## 9.12 n88postfaim

#### Description

Generate tables of standard post-processing quantities.

For discussion of use, see the section on using n88postfaim in the post-processing chapter.

Note that n88postfaim is implemented in python (in tools/postfaim.py), so you can copy it and modify it should you wish to modify the analysis.

#### Usage

n88postfaim [options] input\_file

#### Arguments

Table 9.21: n88postfaim arguments

Argument	Description
help [-h]	Print help and exit.
output_file [-o] arg	Specify an output file. If no output file is specified, output will go to STDOUT.
node_sets [-N] arg	Specify the node sets to use for analysis. The argument should be a list of node set
	names, separated by commas. If not specified, the value will be read from the input
	file.
element_sets [-E] arg	Specify the element sets to use for analysis. The argument should be a list of element
	set names, separated by commas. Each node set must be matched by the
	corresponding set of elements. If not specified, the value will be read from the input
	file.
sets [-s] arg	A convenience option that sets both node_sets and elements_sets. This is only useful
	if corresponding node and element sets are identically named.
rotation_center [-c] arg	Specify the spatial center used for calculation of angular quantities. The argument
	must be given as a triplet of coordinates. If not specified, the value will be read from
	the input file. If not available, no angular quantities will be calculated.
quiet [-q]	Suppress output to terminal (except for error messages).

## 9.13 n88solver (\_sl and \_sp)

Both solvers are documented together, as all command line arguments recognized by n88solver\_sl can also be used with n88solver\_sp.

#### Description (n88solver\_sl)

Solver suitable for small-strain models with linear elastic material definitions.

See the chapter on Solving Linear Problems for discussion of use.

#### Description (n88solver\_sp)

Solver suitable for small-strain models; can solve nonlinear models containing elastoplastic material definitions.

See the chapter on Solving Nonlinear Problems for discussion of us.

#### Usage

n88solver\_sl [options] input\_file
n88solver\_sp [options] input\_file

#### Arguments

#### Table 9.22: n88solver arguments

Argument	Description
help [-h]	Print help and exit.
version [-v]	Print version information and exit.
quiet [-q]	Suppress output to terminal (except for error messages).
license-check [-l]	Print licensing information.
engine [-g] arg (=mt)	Set the solver engine. Valid values are mt for the multi-threaded CPU engine and nv for the nVidia GPU engine. Note that a license from Numerics88 Solutions is required to use the GPU engine.
threads [-t] arg	Set the number of threads for the mt engine. If not specified, the number of threads will be set to one per CPU core on the system, or one thread per 2048 elements, whichever is less.
device [d] arg (=0)	Set the nVidia CUDA device to use (applies only to nv solver). Multiple devices may be specified in a comma delimited list.
precision arg (=double)	Set the floating point precision used. Values: single, mixed, double.
restart [-r]	Do not use the existing solution as initial value.
convergence_tolerance [-e] arg (=1E-6)	Set the convergence measure tolerance. For n88solver_sp, this applies only to the linear iterations.
threshold_window [-w] arg (=4)	Set the threshold window. Thresholds are not considered reached until they remain below the threshold for at least this number of consecutive iterations. For n88solver_sp, this applies only to the linear iterations.
maximum_iterations arg (=30000)	Set maximum number of iterations. For n88solver_sp, this applies only to the linear iterations; note that the count of linear iterations is reset on each plastic iteration.
maximum_plastic_iterations arg (=1000)	Set maximum number of plastic iterations.

The convergence\_tolerance, maximum\_iterations, and maximum\_plastic\_iterations may also be set in

the input file. If present in both the input file as well as specified on the command line as options to n88solver, the options on the command line to n88solver take precedence.

## 9.14 n88tabulate

#### Description

Extract and tabulate values from n88postfaim output files. The result is suitable for importing into a spreadsheet.

Usage

Table 9.23: n88tabulate positional arguments

Option	Description
input_files	n88postfaim output files to process. Any number may be specified, and wildcard
	expansion of * and ? is performed on systems where the shell does not do this.

Table 9.24: n88tabulate optional arguments

Option	Description
-h,help	show this help message and exit
variables VARIABLES, -V	A list of the variables to extract from the input files. Separate variable names with
VARIABLES	commas. See below for a list of valid variable names. If not specified all possible
	variables will be selected (this makes for a very large table).
from FROM, -f FROM	Obtain the list of variables from the first line of a text file. The variable names may
	be separated by any kind of delimiter (white space or commas). Note that an output
	file (from n88tabulate, generated with theheader option) can be used as a
	from argument, in which case the same selection of variables will be used.
header, -H	Print a header line first. May be used even if no input files are specified.
delimiter DELIMITER, -d	Delimiter character to separate columns. Default is a tab ("\t").
DELIMITER	
output_file OUTPUT_FILE, -o	Output file. If not specified, output will go to STDOUT.
OUTPUT_FILE	

For any variables not found in the analysis file, a dash ("-") will be inserted into the output table.

#### Examples

In the following example, every possible variable will be extracted from every file ending in "\_analysis.txt" in the directory. This will result in a very large number of values. The output will be written to the file summary.txt.

n88tabulate -H -o summary.txt \*\_analysis.txt

In the following example, we request the total forces along the z direction on the first two node sets for two different analysis files.

\$ n88tabulate -H -V "filename,fz\_ns1,fz\_ns2" test25a\_analysis.txt test42a\_analysis.txt

filename	tz_nsl	fz_ns2		
test25a_uniaxia	l.n88mod	el	-0.1019E+02	0.1019E+02
test42a_uniaxia	l.n88mod	el	-0.4641E+02	0.4641E+02

The following example is exactly the same, but the output goes to a file.

```
n88tabulate -H -V "filename,fz_ns1,fz_ns2" -o summary.txt test25a_analysis.txt ↔ test42a_analysis.txt
```

Now suppose we want the same selection of variables on a different analysis file, we could do the following. Notice that we are getting the list of variables from the existing file summary.txt.

```
$ n88tabulate -H --from summary.txt test99a_analysis.txt
filename fz_ns1 fz_ns2
test99a_uniaxial.n88model -0.6442E+02 0.6442E+02
```

In the following example, we are interested in the strain energy density, and request some statistical values. We also use a comma as the delimiter.

```
$ n88tabulate -H -d ',' -V "sed_avg,sed_stddev,sed_skew,sed_kurt" analysis.txt
sed_avg,sed_stddev,sed_skew,sed_kurt
0.2990E+00,0.1127E+00,-0.1512E+01,0.8999E+00
```

#### Variables

In the variable list, certain variables can take one or more numeric indices. This is denoted with . For example, for id\_mat%m, actual variable names are id\_mat1 for the first defined material, id\_mat2 for the second defined material, and so on. Similarly for dx\_avg\_ns%n, actual variables names are dx\_avg\_ns1 for the first node set, dx\_avg\_ns2 for the second node set, and so on.

Table 9.25: Variables corresponding to values in table "Model Input"

variable name	value in analysis file table
filename	Filename
num_els	Number of elements
num_nodes	Number of nodes

Refer to Section 6.3.2.1.

#### Table 9.26: Variables corresponding to values in table "Materials"

variable name	value in analysis file table
mats_mats	Number of materials
id_mat%m	The material ID of the m <sup>th</sup> defined material
count_mat%m	Number of elements for the m <sup>th</sup> defined material

Refer to Section 6.3.2.2.

Table 9.27: Variables corresponding to values in table "Post-processing Sets"

variable name	value in analysis file table
num_pp_sets	The number of sets used in post-processing.

Refer to Section 6.3.2.3.

Table 9.28: Variables corresponding to values in table "Strain Energy Density"

variable name	value in analysis file table
sed_avg	average (all materials)
sed_stddev	std_dev (all materials)
sed_skew	skewness (all materials)
sed_kurt	kurtosis (all materials)
sed_min	minimum (all materials)
sed_max	maximum (all materials)
sed_median	median (all materials)
sed_avg_mat%m	average over the m <sup>th</sup> defined material
sed_stddev_mat%m	sed_dev over the m <sup>th</sup> defined material
sed_skew_mat%m	skewness over the m <sup>th</sup> defined material
sed_kurt_mat%m	kurtosis over the m <sup>th</sup> defined material
sed_min_mat%m	minimum over the m <sup>th</sup> defined material
sed_max_mat%m	maximum over the m <sup>th</sup> defined material
sed_median_mat%m	median over the m <sup>th</sup> defined material

Refer to Section 6.3.2.7.

Table 9.29: Variables corresponding to values in table "Von Mises Stress"

variable name	value in analysis file table
svm_avg	average (all materials)
svm_stddev	std_dev (all materials)
svm_skew	skewness (all materials)
svm_kurt	kurtosis (all materials)
svm_min	minimum (all materials)
svm_max	maximum (all materials)
svm_median	median (all materials)
svm_avg_mat%m	average over the m <sup>th</sup> defined material
svm_stddev_mat%m	svm_dev over the m <sup>th</sup> defined material
svm_skew_mat%m	skewness over the m <sup>th</sup> defined material
svm_kurt_mat%m	kurtosis over the m <sup>th</sup> defined material
svm_min_mat%m	minimum over the m <sup>th</sup> defined material
svm_max_mat%m	maximum over the m <sup>th</sup> defined material
svm_median_mat%m	median over the m <sup>th</sup> defined material

Refer to Section 6.3.2.8.

variable name	value in analysis file table
dx_avg_ns%n	The average displacement in the x direction over all nodes in the n <sup>th</sup> node set.
dx_stddev_ns%n	The standard deviation of the displacement in the x direction over all nodes in the n <sup>th</sup>
	node set.
dx_min_ns%n	The minimum displacement in the x direction over all nodes in the n <sup>th</sup> node set.
dx_max_ns%n	The maximum displacement in the x direction over all nodes in the n <sup>th</sup> node set.
dx_median_ns%n	The median displacement in the x direction over all nodes in the n <sup>th</sup> node set.
dy_avg_ns%n	The average displacement in the y direction over all nodes in the n <sup>th</sup> node set.
dy_stddev_ns%n	The standard deviation of the displacement in the y direction over all nodes in the n <sup>th</sup>
	node set.
dy_min_ns%n	The minimum displacement in the y direction over all nodes in the n <sup>th</sup> node set.
dy_max_ns%n	The maximum displacement in the y direction over all nodes in the n <sup>th</sup> node set.
dy_median_ns%n	The median displacement in the y direction over all nodes in the n <sup>th</sup> node set.
dz_avg_ns%n	The average displacement in the z direction over all nodes in the n <sup>th</sup> node set.
dz_stddev_ns%n	The standard deviation of the displacement in the z direction over all nodes in the n <sup>th</sup>
	node set.
dz_min_ns%n	The minimum displacement in the z direction over all nodes in the n <sup>th</sup> node set.
dz_max_ns%n	The maximum displacement in the z direction over all nodes in the n <sup>th</sup> node set.
dz_median_ns%n	The median displacement in the z direction over all nodes in the n <sup>th</sup> node set.

Table 9.30: Variables corresponding to values in table "Nodal Displacements"

Refer to Section 6.3.2.9.

variable name	value in analysis file table
fx_ns%n	The total force in the x direction over all nodes in the n <sup>th</sup> node set.
fx_stddev_ns%n	The standard deviation of the force in the x direction over all nodes in the n <sup>th</sup> node
	set.
fx_min_ns%n	The minimum force in the x direction over all nodes in the n <sup>th</sup> node set.
fx_max_ns%n	The maximum force in the x direction over all nodes in the n <sup>th</sup> node set.
fx_median_ns%n	The median force in the x direction over all nodes in the n <sup>th</sup> node set.
fy_ns%n	The total force in the y direction over all nodes in the n <sup>th</sup> node set.
fy_stddev_ns%n	The standard deviation of the force in the y direction over all nodes in the n <sup>th</sup> node
	set.
fy_min_ns%n	The minimum force in the y direction over all nodes in the n <sup>th</sup> node set.
fy_max_ns%n	The maximum force in the y direction over all nodes in the n <sup>th</sup> node set.
fy_median_ns%n	The median force in the y direction over all nodes in the n <sup>th</sup> node set.
fz_ns%n	The total force in the z direction over all nodes in the n <sup>th</sup> node set.
fz_stddev_ns%n	The standard deviation of the force in the z direction over all nodes in the n <sup>th</sup> node set.
fz_min_ns%n	The minimum force in the z direction over all nodes in the n <sup>th</sup> node set.
fz_max_ns%n	The maximum force in the z direction over all nodes in the n <sup>th</sup> node set.
fz median ns%n	The median force in the z direction over all nodes in the n <sup>th</sup> node set.

Table 9.31: Variables corresponding to values in table "Nodal Forces"

Refer to Section 6.3.2.10.

variable name	value in analysis file table
fx_ns%n_mat%m	The force in the x direction over nodes in the n <sup>th</sup> node set, summed over nodes
	belonging to the m <sup>th</sup> defined material.
fy_ns%n_mat%m	The force in the y direction over nodes in the n <sup>th</sup> node set, summed over nodes
	belonging to the m <sup>th</sup> defined material.
fz_ns%n_mat%m	The force in the z direction over nodes in the n <sup>th</sup> node set, summed over nodes
	belonging to the m <sup>th</sup> defined material.

Table 9.32: Variables corresponding to values in table "Load Sharing"

#### Refer to Section 6.3.2.13.

Table 9.33: Variables corresponding to values in table "Pistoia Failure Load Estimate"

variable name	value in analysis file table
pis_stiffx	The stiffness in the x direction.
pis_stiffy	The stiffness in the y direction.
pis_stiffz	The stiffness in the z direction.
pis_fx_fail	The estimated failure load in the <i>x</i> direction.
pis_fy_fail	The estimated failure load in the <i>y</i> direction.
pis_fz_fail	The estimated failure load in the <i>z</i> direction.

#### Note

The Pistoia Failure Load Estimate table is no longer generated by n88postfaim, but may be generated by the tool n88pistoia if desired. The corresponding variables are by default not included, unless a variable list which includes them is specified.

Refer to Section 8.2 and Section 9.11.

## Chapter 10

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## **Appendix A**

# Loading the Numerics88 plugins for ParaView

The ParaViews plugins are included with the Faim distribution, in the directory ParaView Plugins. They are also distributed separately by Numerics88, as they do not depend on any other part of Faim. If you have obtained them separately, they can be copied to any convenient directory.



#### Important

The ParaView plugins are specific to a particular version of ParaView and can not be loaded into a different version of ParaView. In Faim 7.1, the particular versions of ParaView which are supported depend on the operating system, as follows: - Windows: ParaView 4.4 - OS-X: ParaView 3.14 and 4.2 - Linux: ParaView 3.14, 4.2 and 4.4



#### Important

On Linux and OS-X do not start ParaView from the command line of the same terminal that you run Faim from; the libraries will conflict. Instead, open the file browser and browse to the ParaView installation location (e.g. / opt/ParaView-4.2.0-Linux-64bit/bin on Linux) and start ParaView by double-clicking on the paraview icon.

To load to plugins, open ParaView, and from the Tools menu select Manage Plugins. The Plugin Manager will appear, as shown in Figure A.1.

Name   Property			Name         EyeDomeLightingV         MantaView         Moments         PrismPlugin         PacMan         PointSprite_Plugin         pvblot         SierraPlotTools         SLACTools         StreamingView         SurfaceLIC         H5PartReader         CoProcessingPlugi         AnalyzeNIfTIIO	Property         /iew       Not Loaded         Not Loaded
Load New	Load Selected	Remove	Load New	.oad Selected Remov

Figure A.1: ParaView's Plugin Manager

To load plugins, click the Load New... button and navigate to the location of the plugins (for example /Applications/Faim 7.1/ParaView Plugins/ParaView 4.2 or C:\Program Files\Faim 7.1\ParaView Plugins\ParaVie w 4.4). Select one of the plugins, and then click OK. You will need to repeat this for each of the plugins, in particular for

- libAIMReader,
- libImageGaussianSmooth and
- libN88ModelReader.

They are now loaded, and you should be able to read to corresponding file formats. For more convenient future use, we want to set Auto Load on each of these. To do this, click on the arrow beside the plugin in the Plugin Manager, and make sure that Auto Load is selected. This is shown in Figure A.2.



Figure A.2: Selecting Auto Load in ParaView's Plugin Manager

## **Appendix B**

# Upgrading from previous versions

## B.1 Upgrading from Faim version 6

#### B.1.1 Updating version 6 vtkn88 scripts to work with version 7

vtkn88 is now based on VTK version 6.1. Many of the example scripts in vtkn88 version 6 and earlier used the VTK method SetInput, which has been deprecated and replaced with SetInputData. Simply replacing SetInput with SetInputD ata is sufficient to fix these scripts.

For example, here is a simple operation, in Python, that writes a n88model file. This is the version 6 version:

```
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInput(model)
writer.SetFileName(output_file)
writer.Update()
```

For version 7, it needs to be updated to:

```
writer = vtkn88.vtkn88N88ModelWriter()
writer.SetInputData(model)
writer.SetFileName(output_file)
writer.Update()
```

## B.2 Upgrading from Faim 5

#### B.2.1 Converting Faim version 5 file formats

Faim version 5 used two file formats: .inp files for input files to faim, and .dat files for output. These can be upgraded to version 6 style n88model files with the n88copymodel tool. You may want to upgrade old archived files. Besides being much more space efficient, the new file format is also more robust. It is also standards-compliant, and is more easily read with third party software. (See n88model File Format.)

To convert a version 5 style file, use n88copymodel like this,

n88copymodel olddata.inp newdata.n88model

You can also specify that compression be used in writing the n88model file, like this

n88copymodel --compress olddata.inp newdata.n88model

Compressed n88model files take less disk space, but are slower to read and particularly to write. They are otherwise identical to uncompressed n88model files. You never need to uncompress them before using them.

Version 5 .dat output files are somewhat more problematic to convert to version 6 n88model files, because the .dat files do not contain the complete model information. In particular, they lack any information about material parameters or about boundary conditions or applied loads. Nevertheless, if you have only a .dat file, it is still possible to convert it to a n88model file, but the resulting model will be incomplete. It can be opened and visualized with ParaView, and it is possible to read the solution fields out of it, but it cannot be re-solved, nor can it be processed with n88postfaim.

A .dat file can be converted with

n88copymodel olddata.dat newdata.n88model

As before, you may optionally specify --compress.

If you have both the original .inp and the .dat file, they can be converted to a n88model file by specifying both as input arguments,

n88copymodel olddata.inp olddata.dat newdata.n88model 0

• The order is important: the .inp should be specified first.

This will create a n88model file that can used either as a complete input file to n88solver, should you wish to solve it again, and that also contains the complete solution fields.

#### B.2.2 Updating 5 vtkn88 scripts to work with 6

Here we outline the steps required to update a version 5.x vtkn88 script to work in 6.0. We do not document all the changes and additions to vtkn88 in 6.0, instead we only concentrate on those changes that must be made to get old scripts to work correctly in 6.0

• vtkn88Material instances should be assigned a name.

All materials are now required to have a unique name. In fact, if you don't explicitly set a name, vtkn88 will assign a unique name for you, but it will be an uninformative name such as "NewMaterial1". Names can be assigned like this:

```
bone_material = vtkn88.vtkn88LinearIsotropicMaterial()
bone_material.SetName("bone")
```

• Method SetModelSourceDescription of vtkn88FiniteElementModel is deprecated.

Having this method present will not prevent the scripts from running, but will generate a warning message. The functionality is now encompassed by the Log field of vtkn88FiniteElementModel, which allows a much greater amount of information to be recorded.

• Method NodeIdsFromSelection of vtkn88FiniteElementModel is deprecated.

Use the method GetNodeSet instead.

- Method CreateDisplacementConstraint of vtkn88FiniteElementModel is renamed to ApplyBoundaryCondit ion.
- Method CreateFixedConstraint of vtkn88FiniteElementModel is renamed to FixNodes.
- Method CreateForceConstraint of vtkn88FiniteElementModel is renamed to ApplyLoad.
- Method DataSetFromSelection of vtkn88FiniteElementModel is deprecated.

Use either DataSetFromNodeSet or DataSetFromElementSet.

• Method PolyDataFromSelection of vtkn88FiniteElementModel is deprecated.

#### You can duplicate this functionality as follows. Instead of

```
visible_bone_vertices = model.PolyDataFromSelection("bone_top")
```

the following code can be used instead:

```
reduceToPolyData = vtk.vtkGeometryFilter()
reduceToPolyData.SetInput(model.DataSetFromNodeSet("bone_top"))
reduceToPolyData.MergingOff()
reduceToPolyData.Update()
visible_bone_vertices = reduceToPolyData.GetOutput()
```

Note that this functionality is rarely required, as its main use was to write node sets as VTK PolyData files (which are slightly more efficient than VTK Unstructured Grid files). We now recommend not performing this within scripts at all, but instead to use n88extractsets to extract the node sets from .n88model files.

• The names of node sets (and element sets) must be set on the data array of Point IDs.

#### Instead of this

model.AddNodeSet(visibleNodesIds, "bone\_top")

#### we now write this

```
visibleNodesIds.SetName("bone_top")
model.AddNodeSet(visibleNodesIds)
```

- Class vtkn88FiniteElementRun is renamed to vtkn88SolverParameters .
- Specify element sets as well as node sets for post-processing. For examples, refer to the tutorials on vtkn88, specifically Section 7.6.7 and Section 7.8.13.
- You should make use of the History and Log fields. See any of the tutorials on vtkn88 for examples.
- Instead of vtkn88FAIMInputWriter use vtkn88N88ModelWriter. Don't forget to use a file name extention ".n88model" instead of ".inp".
- Don't specify the iteration limit for the convergence tolerance. If you really want to change these from their defaults, use the command line arguments to n88solver.

## Appendix C

# n88model File Format

The n88model format is a type of NetCDF4/HDF5 file. NetCDF4/HDF5 is a very widely used, high performance and robust file format for scientific and numerical data. Many standard data processing packages are able to read either NetCDF4 or HDF5, which makes it generally straightforward to import Faim data for custom processing.

#### Note

The curious may be wondering how a file can be both NetCDF4 and HDF5. Historically, NetCDF and HDF were different formats. As they served largely similar purposes, starting with NetCDF 4, NetCDF adopted the HDF5 file format (amongst other options), while retaining the familiar NetCDF API or programming interface. Functionally, NetCDF is a subset of HDF5, with a somewhat simpler API. HDF5 files must be structured in a specific way to be a NetCDF4 file; not all HDF5 files can be read through the NetCDF4 library.

## C.1 Converting a n88model file to and from a text file

Sometimes it is useful to examine or modify a data file by hand. Users of faim 5.x may recall that it used a text format, which while subject to certain disadvantages, was easy to edit manually. n88model files cannot be modified directly by hand, however they can be converted to a type of text file, called CDL, that is very concise and human readable. Furthermore, CDL text files, provided they are consistent with the n88model format convention, can easily be converted back into an n88model file.

To convert an n88model file to text, the command ncdump can be used. For example:

ncdump 1x1x2\_uniaxial.n88model > 1x1x2\_uniaxial.txt

#### Note

You can create this example file with the command n88modelgenerator 1x1x2.vti. The file 1x1x2.vti can be found in the data directory of faim. It is a trivial 2-element geometry.

To convert it back again (perhaps after modifying it), follow this example

ncgen -k hdf5 -o 1x1x2\_uniaxial.n88model 1x1x2\_uniaxial.txt

## C.2 Example n88model file in CDL text format

The easiest way to understand the structure of an n88model file is to examine it in text format. Here is the  $1x1x2\_uniaxial$ . txt file, generated in the previous section example. This model has been solved and the file contains solution data. Although it is only two elements, the text representation of the n88model file is rather lengthy!

```
netcdf \1x1x2_uniaxial {
dimensions:
   Dimensionality = 3;
// global attributes:
        :Conventions = "Numerics88/Finite_Element_Model-1.0" ;
        :ActiveProblem = "Problem1" ;
        :Log = "2012-Jul-18 08:59:45\nn88modelgenerator parameters:\n\ninput_file
                                                                                    = / ~
           Applications/faim-6.0/data/1x1x2.vti\noutput_file = 1x1x2_uniaxial.n88model\ ↔
           ntest
                                           = uniaxial\ntest_axis
                                                                                      = z \ ↔
                                           = -0.01 \ln
                                                                                   = off\ ↔
           nstrain
           ntop_surface
                                           = intersection\nbottom_surface
                                                                                          =
                                                                                             \leftarrow
           intersection\nmaterial_table
                                                        = homogeneous\nyoungs_modulus ~
                          = 6829\npoissons_ratio
                                                                 = 0.3\nconnectivity_filter ↔
                      = warn\n\n2012-Jul-18 09:19:26\nn88solver parameters:\n\nengine \ \leftrightarrow
                             = mt\nthreads
                                                            = 1\nrestart
                                                                                            =
                                         = 30000\nconvergence tolerance
                                                                           = 1e-06\nresidual ↔
             0\nlimit
                                                           = 4\n";
            tolerance
                            = 0\nwindow
        :History = "2012-Jul-18 08:59:45 Model created by n88modelgenerator version 6.0 \leftarrow
            n2012-Jul-18 09:19:26 Solved by n88solver version 6.0\n2012-Jul-18 09:19:26 ↔
            Derived fields calculated by n88derivedfields version 6.0";
        :ActiveSolution = "Solution1" ;
group: MaterialDefinitions {
  group: NewMaterial1 {
    // group attributes:
            :Type = "LinearIsotropic" ;
            :E = 6829. ;
            :nu = 0.3 ;
   } // group NewMaterial1
  } // group MaterialDefinitions
group: Parts {
  group: Part1 {
   dimensions:
        NumberOfNodes = 12 ;
    variables:
        float NodeCoordinates(NumberOfNodes, Dimensionality);
   data:
    NodeCoordinates =
  0, 0, 0,
  1, 0, 0,
  0, 1, 0,
  1, 1, 0,
  0, 0, 1,
  1, 0, 1,
  0, 1, 1,
  1, 1, 1,
  0, 0, 2,
  1, 0, 2,
  0, 1, 2,
  1, 1, 2;
    group: Elements {
```

```
group: Hexahedrons {
   dimensions:
```

```
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```

```
NumberOfNodesPerElement = 8 ;
           NumberOfElements = 2 ;
        variables:
            uint ElementNumber(NumberOfElements) ;
            uint NodeNumbers(NumberOfElements, NumberOfNodesPerElement) ;
            ushort MaterialID(NumberOfElements) ;
        data:
         ElementNumber = 1, 2;
        NodeNumbers =
  1, 2, 3, 4, 5, 6, 7, 8,
  5, 6, 7, 8, 9, 10, 11, 12;
        MaterialID = 127, 127;
        } // group Hexahedrons
      } // group Elements
    group: MaterialTable {
     dimensions:
        Size = 1;
      variables:
       ushort ID(Size) ;
       string MaterialName(Size) ;
      data:
       ID = 127;
      MaterialName = "NewMaterial1" ;
      } // group MaterialTable
    } // group Part1
  } // group Parts
group: Constraints {
  group: bottom_fixed {
   dimensions:
       NumberOfValues = 4;
    variables:
        uint NodeNumber(NumberOfValues) ;
       byte Sense(NumberOfValues) ;
       float Value(NumberOfValues) ;
    // group attributes:
            :Part = "Part1" ;
            :Type = "NodeAxisDisplacement" ;
    data:
    NodeNumber = 1, 2, 3, 4;
    Sense = 3, 3, 3, 3;
    Value = 0, 0, 0, 0;
    } // group bottom_fixed
  group: top_displacement {
    dimensions:
       NumberOfValues = 4 ;
    variables:
        uint NodeNumber(NumberOfValues) ;
        byte Sense(NumberOfValues) ;
        float Value(NumberOfValues) ;
```

```
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```

```
// group attributes:
            :Part = "Part1" ;
            :Type = "NodeAxisDisplacement" ;
    data:
    NodeNumber = 9, 10, 11, 12;
    Sense = 3, 3, 3, 3;
    Value = -0.02, -0.02, -0.02, -0.02;
    } // group top_displacement
  } // group Constraints
group: Sets {
 group: NodeSets {
   group: face_z0 {
     dimensions:
       NumberOfNodes = 4 ;
      variables:
       uint NodeNumber(NumberOfNodes) ;
      // group attributes:
           :Part = "Part1" ;
      data:
      NodeNumber = 1, 2, 3, 4;
      } // group face_z0
   group: face_z1 {
     dimensions:
       NumberOfNodes = 4 ;
      variables:
       uint NodeNumber(NumberOfNodes) ;
      // group attributes:
           :Part = "Part1" ;
      data:
      NodeNumber = 9, 10, 11, 12;
      } // group face_z1
    group: face_x0 {
      dimensions:
       NumberOfNodes = 6 ;
     variables:
       uint NodeNumber(NumberOfNodes) ;
      // group attributes:
           :Part = "Part1" ;
      data:
      NodeNumber = 1, 3, 5, 7, 9, 11;
      } // group face_x0
    group: face_x1 {
     dimensions:
        NumberOfNodes = 6;
      variables:
       uint NodeNumber(NumberOfNodes) ;
```

```
// group attributes:
         :Part = "Part1" ;
    data:
    NodeNumber = 2, 4, 6, 8, 10, 12;
   } // group face_x1
 group: face_y0 {
   dimensions:
     NumberOfNodes = 6 ;
    variables:
     uint NodeNumber(NumberOfNodes) ;
    // group attributes:
         :Part = "Part1" ;
    data:
    NodeNumber = 1, 2, 5, 6, 9, 10;
   } // group face_y0
 group: face_y1 {
   dimensions:
     NumberOfNodes = 6 ;
   variables:
     uint NodeNumber(NumberOfNodes) ;
    // group attributes:
        :Part = "Part1" ;
   data:
    NodeNumber = 3, 4, 7, 8, 11, 12;
    } // group face_y1
  } // group NodeSets
group: ElementSets {
 group: face_z0 {
   dimensions:
     NumberOfElements = 1 ;
   variables:
     uint ElementNumber(NumberOfElements) ;
    // group attributes:
         :Part = "Part1" ;
   data:
    ElementNumber = 1 ;
   } // group face_z0
 group: face_z1 {
   dimensions:
     NumberOfElements = 1 ;
   variables:
     uint ElementNumber(NumberOfElements) ;
    // group attributes:
         :Part = "Part1" ;
    data:
    ElementNumber = 2;
    } // group face_z1
```

```
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```

```
group: face_x0 {
     dimensions:
       NumberOfElements = 2 ;
     variables:
       uint ElementNumber(NumberOfElements) ;
      // group attributes:
           :Part = "Part1" ;
      data:
      ElementNumber = 1, 2;
      } // group face_x0
    group: face_x1 {
     dimensions:
       NumberOfElements = 2 ;
      variables:
       uint ElementNumber(NumberOfElements) ;
      // group attributes:
            :Part = "Part1" ;
      data:
      ElementNumber = 1, 2;
      } // group face_x1
    group: face_y0 {
     dimensions:
       NumberOfElements = 2 ;
      variables:
       uint ElementNumber(NumberOfElements) ;
      // group attributes:
           :Part = "Part1" ;
      data:
      ElementNumber = 1, 2 ;
      } // group face_y0
    group: face_y1 {
     dimensions:
       NumberOfElements = 2 ;
     variables:
       uint ElementNumber(NumberOfElements) ;
      // group attributes:
            :Part = "Part1" ;
      data:
      ElementNumber = 1, 2 ;
      } // group face_y1
    } // group ElementSets
  } // group Sets
group: Problems {
 group: Problem1 {
    // group attributes:
            :Part = "Part1" ;
            :Constraints = "bottom_fixed,top_displacement" ;
```

```
:PostProcessingNodeSets = "face_z1, face_z0" ;
            :PostProcessingElementSets = "face_z1, face_z0" ;
            :RotationCenter = 0.5, 0.5, 1. ;
    } // group Problem1
  } // group Problems
group: Solutions {
  group: Solution1 {
    // group attributes:
            :Problem = "Problem1" ;
    group: NodeValues {
      dimensions:
        NumberOfNodes = 12 ;
      variables:
        float Displacement(NumberOfNodes, Dimensionality);
        float Residual(NumberOfNodes, Dimensionality);
        float ReactionForce(NumberOfNodes, Dimensionality);
      data:
       Displacement =
  -0.001500001, -0.001500001, 0,
  0.001500001, -0.001500001, 0,
  -0.001500001, 0.001500001, 0,
  0.001500001, 0.001500001, 0,
  -0.001500001, -0.001500001, -0.01000001,
  0.001500001, -0.001500001, -0.01000001,
  -0.001500001, 0.001500001, -0.01000001,
  0.001500001, 0.001500001, -0.01000001,
  -0.001500001, -0.001500001, -0.02,
  0.001500001, -0.001500001, -0.02,
  -0.001500001, 0.001500001, -0.02,
  0.001500001, 0.001500001, -0.02;
       Residual =
  -1.528847e-07, -1.528847e-07, 0,
  1.528847e-07, -1.528847e-07, 0,
  -1.528847e-07, 1.528847e-07, 0,
 1.528847e-07, 1.528847e-07, 0,
 1.437116e-05, 1.437116e-05, 3.424616e-05,
  -1.437116e-05, 1.437116e-05, 3.424616e-05,
 1.437116e-05, -1.437116e-05, 3.424616e-05,
  -1.437116e-05, -1.437116e-05, 3.424616e-05,
 1.452404e-05, 1.452404e-05, 0,
  -1.452404e-05, 1.452404e-05, 0,
  1.452404e-05, -1.452404e-05, 0,
  -1.452404e-05, -1.452404e-05, 0 ;
       ReactionForce =
  1.528847e-07, 1.528847e-07, 17.07251,
  -1.528847e-07, 1.528847e-07, 17.07251,
  1.528847e-07, -1.528847e-07, 17.07251,
  -1.528847e-07, -1.528847e-07, 17.07251,
  -1.437116e-05, -1.437116e-05, -3.424616e-05,
  1.437116e-05, -1.437116e-05, -3.424616e-05,
-1.437116e-05, 1.437116e-05, -3.424616e-05,
  1.437116e-05, 1.437116e-05, -3.424616e-05,
  -1.452404e-05, -1.452404e-05, -17.07248,
  1.452404e-05, -1.452404e-05, -17.07248,
 -1.452404e-05, 1.452404e-05, -17.07248,
```

```
1.452404e-05, 1.452404e-05, -17.07248;
    } // group NodeValues
 group: ElementValues {
   dimensions:
     NumberOfElements = 2 ;
     NumberOfStressStrainComponents = 6 ;
    variables:
      float Stress(NumberOfElements, NumberOfStressStrainComponents) ;
     float VonMisesStress(NumberOfElements) ;
      float Strain(NumberOfElements, NumberOfStressStrainComponents) ;
      float StrainEnergyDensity(NumberOfElements);
    data:
     Stress
-6.115387e-07, -6.115387e-07, -68.29005, 0, 0, 0,
5.809617e-05, 5.809617e-05, -68.28991, 0, 0, 0;
    VonMisesStress = 68.29005, 68.28997 ;
    Strain =
0.003000002, 0.003000002, -0.01000001, 0, 0, 0,
0.003000002, 0.003000002, -0.009999992, 0, 0, 0;
    StrainEnergyDensity = 0.3414505, 0.3414495 ;
    } // group ElementValues
  } // group Solution1
} // group Solutions
```

## C.3 Specification

NetCDF4 files consist of dimensions, variables and attributes, as well as groups. Groups can contain dimensions, variables and attributes, as well as other groups, thus forming a nested tree structure. Variables can also contain attributes.

Types specified below as "numeric" may be any concrete numeric type. Similarly "integral" may be any concrete integer type.

It is convenient to refer to the text format example when trying to follow the file specification.

#### Note

}

In some cases dimensions may be named differently than specified below. (For complex reasons some of the n88 tools are unable to deduce the correct dimension names in certain rare cases.) This should be avoided where possible when writing a file. For reading files, the most reliable method is to read the dimensions of the corresponding variables, rather than looking up dimensions in the file by name.

#### C.3.1 Root group

The root group exists for all NetCDF4 files. It does not need to be created.

#### attribute Conventions [text]

Specifies that this is a n88model file. Must be "Numerics88/Finite\_Element\_Model-1.0". Required.

#### attribute ActiveProblem [text]

Specifies the problem that will be used as input to the solver. Must be set to a name of a subgroup of the *Problems* group. Required by the solver.

#### attribute ActiveSolution [text]

Specifies the active solution set, which is typically the one that will be used for post-processing or rendering. Must be set to a name of a subgroup of the *Solution* group. Required by n88postfaim, but not required by the solver.

#### attribute *History* [text]

Brief history of the operations that have been performed on the file. By convention, add one line to the history for each operation performed on the file. Each line should start with a time/date stamp. Additional detail should go into the *Log* attribute. Required.

#### attribute Log [text]

As much additional detail as required about operations that have been performed on the file. Each addition or section in *Log* may be multiple lines. It is recommended that each section start with a time/date stamp, in order to make it easy to correlate with *History*. Optional.

#### dimension Dimensionality [text]

Specifies the dimension of the problem. Currently it must be 3, although future versions of Faim might also support 2D models. Required.

#### C.3.2 MaterialDefinitions group

This group contains material definitions. Each material definition is implemented as a subgroup, where the name of the subgroup is the name of the material being defined. Each subgroup is required to have an attribute *Type*. Required.

#### subgroups of MaterialDefinitions of Type "LinearIsotropic"

A subgroup that defines a linear isotropic material. Optional. As many may be defined as required.

## attribute Type [text]

"LinearIsotropic". Required.

#### attribute *E* [numeric]

Specifies the Young's Modulus of the material. Required.

#### attribute nu [numeric]

Specifies the Poisson's Ratio of the material. Required.

#### subgroups of MaterialDefinitions of Type "LinearOrthotropic"

A subgroup that defines a linear orthotropic material. Optional. As many may be defined as required.

attribute Type [text]

"LinearOrthotropic". Required.

attribute *E* [numeric, length 3]

Specifies the Young's Modulii of the material as  $E_{xx}$ ,  $E_{yy}$ ,  $E_{zz}$ . Required.

attribute *nu* [numeric, length 3] Specifies the Poisson's Ratio of the material as  $v_{yz}$ ,  $v_{zx}$ ,  $v_{xy}$ . Required.

attribute *G* [numeric, length 3]

Specifies the Shear Modulus of the material as  $G_{yz}$ ,  $G_{zx}$ ,  $G_{xy}$ . Required.

#### subgroups of MaterialDefinitions of Type "LinearAnisotropic"

A subgroup that defines a linear anisotropic material. Optional. As many may be defined as required.

#### attribute Type [text]

"LinearAnisotropic". Required.

#### attribute StiffnessMatrix [numeric, length 36]

Specifies the 36 elements of the stiffness matrix. Note that since the stiffness matrix is symmetric, there are only 21 unique values, but all 36 must be given. They must be specified in the order  $K_{11}$ ,  $K_{12}$ ,  $K_{13}$ ...  $K_{66}$ , but since the matrix is symmetric, this is equivalent to  $K_{11}$ ,  $K_{21}$ ,  $K_{31}$ ...  $K_{66}$ . Required.

#### subgroups of MaterialDefinitions of Type "VonMisesIsotropic"

A subgroup that defines an isotropic von Mises elastoplastic material. Optional. As many may be defined as required.

#### attribute *Type* [text]

"LinearIsotropic". Required.

**attribute** *E* **[numeric]** Specifies the Young's Modulus of the material. Required.

attribute nu [numeric]

Specifies the Poisson's Ratio of the material. Required.

#### attribute *Y* [numeric]

Specifies the Yield Strength of the material. Required.

#### subgroups of MaterialDefinitions of Type "MohrCoulombIsotropic"

A subgroup that defines an isotropic Mohr Coulomb elastoplastic material. Optional. As many may be defined as required.

attribute *Type* [text]

"LinearIsotropic". Required.

#### attribute E [numeric]

Specifies the Young's Modulus of the material. Required.

#### attribute *nu* [numeric]

Specifies the Poisson's Ratio of the material. Required.

#### attribute *c* [numeric]

Specifies the Mohr Coulomb *c* parameter (cohesion) of the material. Required.

#### attribute *phi* [numeric]

Specifies the Mohr Coulomb  $\varphi$  parameter (friction angle) of the material. Required.

#### attribute psi [numeric]

Specifies the Mohr Coulomb  $\psi$  parameter (dilation angle) of the material. Optional, assumed zero if not specified.

#### C.3.3 Parts group

This group defines parts. A part is a geometric collection of elements, along with the associated nodes and the material assignments for the elements. Each part is implemented as a subgroup, where the name of the subgroup is the name of the part being defined.

#### subgroups of Part

The subgroup name gives the part name. At least one subgroup is required, and multiple ones may be defined.

#### dimension NumberOfNodes

The number of nodes in the variable NodeCoordinates.

#### variable NodeCoordinates (NumberOfNodes, Dimensionality) [numeric]

Specifies the x,y,z coordinates of the nodes. The node numbering is implicit, and 1-based. Hence the first row is node 1, the second node 2, etc...

#### subgroup MaterialTable of subgroups of Part

Maps material names, as defined in *MaterialDefinitions*, to material ID numbers. Material ID numbers are then assigned to each element. Required by the solver.

#### dimension Size

The number of entries in the material table for this part.

#### variable MaterialName (Size) [text]

The material names, corresponding to subgroups in *MaterialDefinitions*. Required.

#### variable *ID* (Size) [integral]

The IDs assigned to to materials. Any IDs in the range 1-32768 may be assigned, provided they are unique. Required.

#### subgroup Element of subgroups of Part

Required. Currently must itself contain exactly the single subgroup, Hexahedrons.

#### subgroup Hexahedron of subgroup Element of subgroups of Part

Defines the hexahedral elements of the part. Note that the current version of n88solver only handles regular hexahedrons, although the file format does not enforce this. Currently required, although in future versions supporting multiple element types, may become optional.

#### dimension NumberOfNodesPerElement [=8]

The number of nodes per element, which for hexahedrons is 8.

#### dimension NumberOfElements

The number of hexahedral elements.

#### variable *ElementNumber* (NumberOfElements) [integral]

Explicitly assigned element numbers. In the current version, the solver requires consecutively-numbered elements starting with element 1, but this restriction may be relaxed in future versions. Required.

#### variable NodeNumbers (NumberOfElements, NumberOfNodesPerElement)

The node numbers of the nodes defining each hexahedron. The topology is as the VTK type VTK\_VOXEL, and is shown in Figure C.1. The global node numbers (1-indexed) must be given for each element in the order as shown in the figure. Required.

#### variable MaterialID (NumberOfElements) [integral]

The material IDs of the materials assigned to each element. IDs correspond to values in the MaterialTable for this part. Required.



Figure C.1: Topology of hexahedral elements in n88model file (1-indexed).

#### Warning

The ordering of the elements in the input file has a strong influence on the solver. Certain orderings are optimal and will solve in the fastest time. There exist orderings which will cause the solver to fail with an error. A future version of Faim might reorder the input elements as required, but in the current version, we strongly recommend that elements be ordered in the file according to "x fastest, z slowest".

### C.3.4 Constraints group

Constraints are sets of values assigned to nodes, and used to define both boundary conditions and applied loads. Each constraint (which itself is a set of values) is implemented as a subgroup, where the name of the subgroup is the name of the constraint being defined. Optional, although a well-defined problem will always have some constraints.

#### Note

vtkn88 supports constraints defined on elements as well, which the n88model file format does not currently support. This is the natural way to define applied loads. The file writers in vtkn88 distribute element forces appropriately on to the nodes on writing. Because of this, vtkn88N88ModelWriter and vtkn88N88ModelReader are not quite inverses. Using them in sequence can result in a model with a different, although physically equivalent, set of constraints.

#### subgroups of Constraints

The subgroup name gives the Constraint name. Optional. Any number of subgroups may be defined.

#### attribute Part [text]

The part to which the constraint is associated. Note that this does not necessarily imply that the constraint will in fact be applied to the named part. Refer to the attribute *Constraints* in the *Problems* group.

#### attribute Type [text]

Currently two types are supported, *NodeAxisDisplacement* and *NodeAxisForce*. For the former, specific displacements for given nodes along given axis directions (the "sense") are defined. The latter is similar but the specified values are forces.

#### dimension NumberOfValues

The number of values specified by this constraint.

variable NodeNumber (NumberOfValues) [integral]

A list of the node numbers to which the constraint is applied.

#### variable Sense (NumberOfValues) [integral]

A list of the senses along which the constraint is applied. Valid values are 1,2,3 for x,y,z respectively.

#### variable Value (NumberOfValues) [integral]

A list of the values (displacement or force) of the constraint.

#### C.3.5 Sets group

Sets are collections of nodes or of elements. The primary use of sets in n88model files is for post-processing. n88postfaim requires at least two-post processing sets of nodes, which must be matched by sets of the corresponding elements. Quantities (*e.g.* the difference between the sum of the forces on the node sets) are then calculated between pairs of sets. A secondary use of sets is simply to store sets that can be further refined and transformed into boundary conditions during model generation. This is particularly useful when the model generation occurs in several stages.

#### subgroup NodeSets of Sets

Defines node sets. Each node set is implemented as a subgroup, where the name of the subgroup is the name of the node set being defined. Required by n88postfaim.

#### subgroups of subgroup NodeSets of Sets

The subgroup name gives the node set name. Optional. As many may be defined as required.

#### attribute Part [text]

The part with which the node set is associated.

#### dimension NumberOfNodes

The number of nodes in the node set.

#### variable NodeNumber

A list of the node numbers of the nodes in the set.

#### subgroup *ElementSets* of *Sets*

Defines element sets. Each element set is implemented as a subgroup, where the name of the subgroup is the name of the element set being defined. Optional, although element sets must be defined if n88postfaim is to be used.

#### subgroups of subgroup *ElementSets* of *Sets*

The subgroup name gives the element set name. Optional. As many may be defined as required.

#### attribute Part [text]

The part with which the element set is associated.

#### dimension NumberOfElements

The number of elements in the element set.

#### variable *ElementNumber*

A list of the element numbers of the elements in the set.

#### C.3.6 Problems group

The *Problems* group defines problems that can be solved by the solver. Multiple problems may be defined. Each problem is implemented as a subgroup, where the name of the subgroup is the name of the problem being defined. In the current version, only the problem specified by the root-level attribute *ActiveProblem* will be solved when the file is submitted to the solver. Required by the solver.

#### subgroups of Problem

The subgroup name gives the problem name. Optional. As many may be defined as required.

#### attribute Part [text]

Gives the part that will be used for this problem. Required.

#### attribute Constraints [text]

Gives a list of constraints that will be applied to the problem. Takes the form of a list of constraint names separated by commas. It is clearly a logical error to assign constraints that are associated with a different part. Required.

#### attribute ConvergenceTolerance [numeric]

Specifies the convergence tolerance to be used by the solver. Optional, and recommended that you not set this in the n88model file, because the optimum value depends on the solver. The solver will typically choose an appropriate value, but the choice can be specified with a command line option to n88solver, which is the recommended way to set the convergence tolerance should you wish to change it.

#### attribute ResidualTolerance [numeric]

Specifies the residual tolerance to be used by the solver. Optional, and recommended that you not set this in the n88model file, because the optimum value depends on the solver. The solver will typically choose an appropriate value, but the choice can be specified with a command line option to n88solver, which is the recommended way to set the residual tolerance should you wish to change it.

#### attribute MaximumIterations [integral]

Specifies the maximum iterations to be used by the solver. Optional, and recommended that you not set this in the n88model file, because the optimum value depends on the solver. The solver will typically choose an appropriate value, but the choice can be specified with a command line option to n88solver, which is the recommended way to set the maximum iterations should you wish to change it.

#### attribute PostProcessingNodeSets [text]

Gives a list of node sets that will be used for post-processing. Takes the form of a list of node set names separated by commas. n88postfaim requires that at least two post-processing node sets to be defined. n88postfaim has an equivalent command-line option which takes precedence.

#### attribute PostProcessingElementSets [text]

Gives a list of element sets that will be used for post-processing. Takes the form of a list of element set names separated by commas. n88postfaim requires that every node set specified in *PostProcessingNodeSets* be exactly matched with an element set of the associated elements. n88postfaim has an equivalent command-line option which takes precedence.

#### attribute RotationCenter (3) [numeric]

Gives the rotation center. This value is used only for post-processing. Optional.

### C.3.7 Solutions group

The solutions group contains solution values as calculated by n88solver or n88derivedfields. Any number of solution sets may be defined (including multiple solution sets per problem). Each solution set is implemented as a subgroup, where the name of the subgroup is the name of the problem being defined. The solution set specified by the root level attribute *ActiveSolution* is the one that will be used for post-processing.

#### subgroups of Solutions

The subgroup name gives the solution set name. Optional. As many may be defined as required.

#### attribute Problem [text]

The problem to which the solution applies. Required.

#### subgroup NodeValues of subgroups of Solutions

A group containing variables that specify values on each node. Variables are identified by name, and may be either onedimensional (scalar values on the nodes), or two-dimensional (vector values on the nodes).

#### dimension NumberOfNodes

The number of nodes in the problem. This is redundant with the number of nodes defined in the part, and must be equal to it. (The NetCDF4 format requires that it be re-defined here.) Required.

#### typical variables in NodeValues

- Displacement (NumberOfNodes, Dimensionality)
- Residual (NumberOfNodes, Dimensionality)
- *ReactionForce* (NumberOfNodes, Dimensionality)

#### subgroup ElementValues of subgroups of Solutions

A group containing variables that specify values on each element. Variables are identified by name, and may be either one-dimensional (scalar values on the elements), or two-dimensional (vector values on the elements).

#### dimension NumberOfElements

The number of elements in the problem. This is redundant with the number of elements defined in the part, and must be equal to it. (The NetCDF4 format requires that it be re-defined here.) Required.

#### dimension NumberOfStressStrainComponents [=6]

Stress and strain are defined on the elements, and have 6 components, so a dimension equal to 6 must be defined. The order must be xx,yy,zz,yz,zx,xy.

#### typical variables in *ElementValues*

- Stress (NumberOfElements, NumberOfStressStrainComponents)
- Strain (NumberOfElements, NumberOfStressStrainComponents)
- VonMisesStress (NumberOfElements)
- *StrainEnergyDensity* (NumberOfElements)

## C.4 Writing code to read and write n88model files

The easiest way to read and write n88model files is through the vtkn88 classes vtkn88N88ModelReader and vtkn88N 88ModelWriter. However, should you wish to avoid the use of vtkn88 for some reason, a couple of other possibilities exist.

The faim distribution includes the NetCDF4 libraries and header files so that it is available to users wishing to write custom applications for handling n88model data. Refer to http://www.unidata.ucar.edu/software/netcdf/docs/ for documentation on using the NetCDF interface.

Faim also includes the python interface netcdf4-python (http://code.google.com/p/netcdf4-python/). Some Numerics88 tools make use of this interface. For an example, have a look at the python script tools/modelinfo.py, which implements the n88modelinfo utility.
# Appendix D

# Automating the Processing of Multiple Models With Scripts



Important

This section currently applies only to OS-X and Linux.

Very often one has not just a single model to solve, but a whole series of data sets that needs to be modelled by FE analysis. The section will show how to use simple shell scripts to automate this task.

#### Tip

We highly recommend initially running the models one at a time, and visualizing the results as you go, to ensure that your models and results are reasonable and as you expect, before sending hundreds of models to be solved in a batch script.

#### Note

Shell scripts are a standard part of any Unix-based operating system, including OS-X. If you want to learn more about shell scripting than we present here, there are many good tutorials on the web. Search for "bash scripting tutorial".

# D.1 A script to generate a mesh and solve it

The first step to is to make a script that can generate a mesh, solve it, and clean up, all with one command. The following shell script does this. You can find a copy of it, named mesh\_solve\_analyze in the examples/batch\_processing directory of the distribution. Alternatively, you can just copy and paste the commands below into a text editor and save it to a file named mesh\_solve\_analyze.

```
#!/bin/bash
#
# This is a simple script that takes a segmented image file name as input,
# generates a finite element model using n88modelgenerator, then solves
# it with the FAIM solver.
#
# Assuming this script is in the current directory, it can be run as follows:
#
./mesh_solve_analyze image_file config_file
#
```

```
# where image file is the segmented image file to be processed, and
# config_file is an n88modelgenerator configuration file.
#
# You may want to edit this script in order to customize it.
if [ $# -ne 2 ] ; then
 echo "Usage: mesh_solve_analyze image_file config_file"
 exit 1
fi
INPUT_IMAGE_FILE="$1"
MODEL_GENERATOR_CONFIG_FILE="$2"
# Strip off the extension of the input file
ROOT_FILE_NAME=`echo "${INPUT_IMAGE_FILE}" | sed 's/\(.*\)\..*/\1/'`
MODEL_FILE="${ROOT_FILE_NAME}.n88model"
date
echo
          ==== Generating ${MODEL_FILE} ===="
echo "
echo
n88modelgenerator --config="${MODEL_GENERATOR_CONFIG_FILE}" \
   "${INPUT_IMAGE_FILE}" "${MODEL_FILE}"
if [ $? -ne 0 ] ; then
 echo "Mesh generation returned error."
  exit 1
fi
echo
echo "
          ==== Solving and post-processing FE model ===="
echo
faim "${MODEL_FILE}"
if [ $? -ne 0 ] ; then
 echo "faim returned error."
  exit 1
fi
echo
echo "
         ==== Compressing data file ===="
echo
n88compress "${MODEL_FILE}"
if [ $? -ne 0 ] ; then
 echo "compress returned error."
 exit 1
fi
echo
```

If this script does exactly what you want, it can be run directly from the installation directory, like this:

/Applications/faim-6.0/examples/batch\_processing/mesh\_solve\_analyze input\_file config\_file

On Linux, Faim is typically installed in /opt rather than /Applications.

where input\_file is the segmented image file to be processed, and config\_file is an n88modelgenerator configuration file. See Section 2.1 for information on the configuration file format. The very simplest configuration file might contain just a single line specifying the test type: test = uniaxial

You can use a text editor to create this file, and save it, for example, as myconfig.conf in your working directory.

You can also copy this script to your working data directory and customize it to your preferences. In this case you would most likely run it like this:

./mesh\_solve\_analyze input\_file config\_file

As a tiny little tutorial, you may want to try to following:

- 1. Copy mesh\_solve\_analyze to your working directory.
- 2. Copy test25a.aim from the data subdirectory of your installation to your working directory.
- 3. Create myconfig.conf as above using a text editor, and save it to your working directory.
- 4. Run mesh\_solve\_analyze:

```
./mesh_solve_analyze test25a.aim myconfig.conf
```

#### Note

The script must be made "executable" before it can be run. The script in the example directory should already be executable, but if you write your own, you may need to change permissions to make it executable before the script can be run:

chmod +x mesh\_solve\_analyze

Some further notes about this script:

## D.2 Scripting several models

Now that we have a command to do everything required for a single data set, we can write a very simple script that will call it several times for a number of different data sets.

Here is an example. Open a text editor and copy in the following lines. Of course, you should replace mydatal.aim, etc... with real data file names. Save it for example as runjobs.sh.

source /Applications/faim-6.0/setenv.sh
./mesh\_solve\_analyze mydata1.aim myconfig.conf
./mesh\_solve\_analyze mydata2.aim myconfig.conf
./mesh\_solve\_analyze mydata3.aim myconfig.conf

It can now be run with this command:

bash runjobs.sh

Tip

Alternatively, you can make it executable with

chmod +x runjobs.sh

and then run it like this:

./runjobs.sh

## **D.3 Unattended execution of scripts**

One issue when running scripts or very long jobs is that if the Terminal in which they were started is closed, or the user logs out, the execution will stop. This is obviously undesirable. The solution is to prepend "nohup" to the command. For example:

nohup bash runjobs.sh

Now it will keep running until completed or manually stopped.

#### Tip

The etymology of nohup is that is is derived from "No Hang Up", which may help to remember it.

However, if you try this, you will note that the messages that usually appear in the Terminal to keep you informed of progress no longer appear. Where did that go? Well, the command has been "detached" from the Terminal window so it can outlive the Terminal. nohup instead will send all the output messages ("STDOUT" in Unix jargon) to a file named nohup.out. You can choose to send it to a file of your choice like this:

nohup bash runjobs.sh &> runjobs.out

As well, since nothing is being output to the Terminal, you might as well get the prompt back so you can continue to use the Terminal for other purposes. Just add an ampersand to the end of the command line, like this:

nohup bash runjobs.sh &> runjobs.out &

Now you can examine runjobs.out as you like, for example with the command:

cat runjobs.out

However, it may be inconvenient to keep re-running this command if you want to monitor the progress in real time. There is a command for that too though:

tail -f runjobs.out

Here the -f flag means "follow". The will continue to echo new lines as they are added to runjobs.out . When you tire of watching this, just hit CONTROL-C. This only stops the tail command; runjobs.sh continues to execute.

Finally, when you start a process with nohup, you may need to know how to stop it as well. If the original Terminal is still open, this is not too difficult. First find the job number with the jobs command:

\$ jobs
[1]+ Running nohup ./runjobs.sh >&runjobs.out &

(Note that the \$ is the command prompt - shown here to distinguish the input from the output. Don't type the \$ character.) In this example, the job number is 1. It can be stopped with the command

kill %1

If the original Terminal is no longer open, then it gets a little more complicated, because we will need to find the Process ID (which is system wide) instead of the Job ID (which is specific to the Terminal). This command will do it in most cases:

\$ ps -A | grep runjobs.sh 55713 ttys007 0:00.00 sh ./runjobs.sh 55719 ttys007 0:00.00 grep runjobs.sh

The Process ID in this example is 55713. We can kill that process with

kill 55713

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# Chapter 11

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