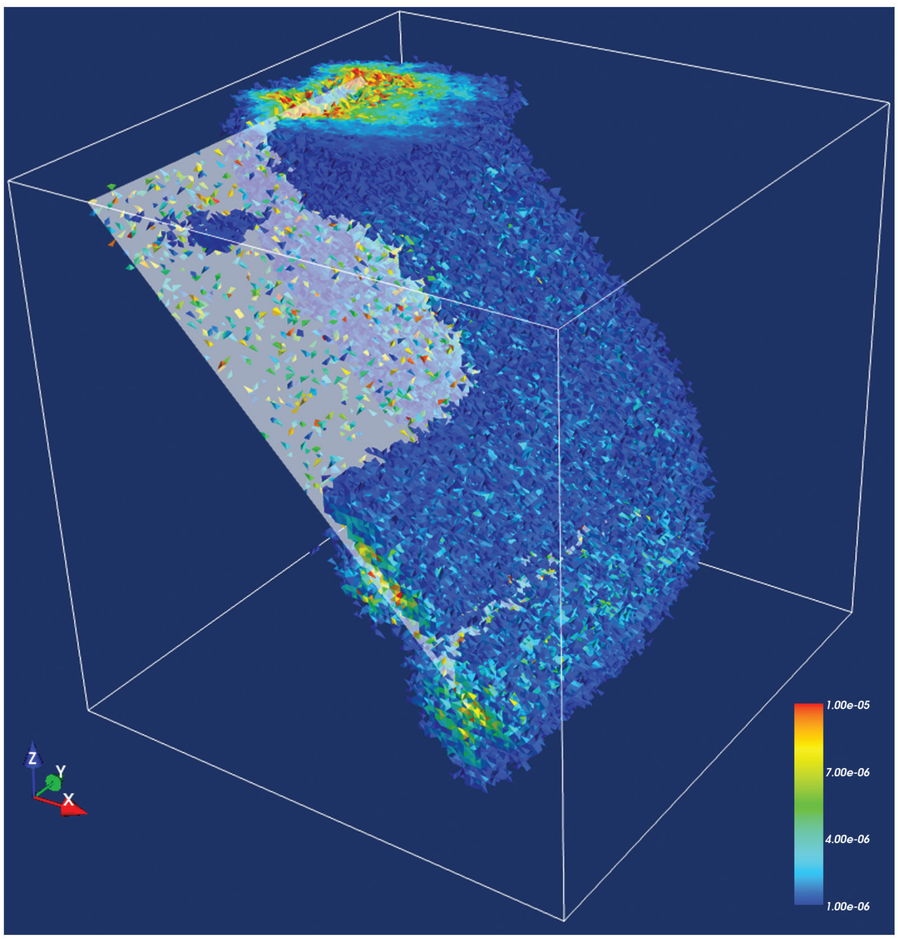
COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)

Cigma

User Manual
Version 0.9



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Cigma

Version 0.9

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Chapter 1

Introduction

1.1 About Cigma

The CIG Model Analyzer (Cigma) consists of a suite of tools intended to facilitate the comparison of numerical models. CIG has developed Cigma in response to demand from the short-term tectonics community for a simple tool that can perform rigorous error analysis on their FEM codes. The long-term goal for Cigma, however, is for it to be used for nearly all geodynamics modeling codes.

In general, Cigma is intended for three types of tasks, namely (1) error analysis, (2) benchmarking, and (3) code verification.

There are two ways in which Cigma can help you with error analysis. It can take a random sampling of points inside a domain of interest and analyze the pointwise differences between physical fields, or otherwise perform an integration of the errors over a discretized version of the domain. This comparison can take place even when the meshes are not compatible.

In benchmarking, Cigma can help the geodynamics community agree on a standard solution to specific problems by facilitating the process of comparing different numerical codes against each other.

Lastly, as an automated tool, Cigma can help developers in creating regression tests to ensure that software changes do not affect the consistency of the results.

At its core, Cigma draws from a variety of libraries, particularly the Tetrahedral Mesh Comparator (TMC) (`www.sci.utah.edu/~bavoil/research/tetsimp/tmc/`) from the University of Utah, which itself draws from the GTB Graphics Toolbox library (`sf.net/projects/gtb`). Cigma extends and generalizes the functionality therein to handle other types of elements as well as adding the ability to compare vector fields.

1.2 Citation

Computational Infrastructure for Geodynamics (CIG) is making this source code available to you in the hope that the software will enhance your research in geophysics. This is a brand-new code and at present no papers are published or at press for use as citations other than this manual, which is cited as follows:

> Armendariz, L., and S. Kientz. *Cigma User Manual.* Pasadena, CA: Computational Infrastructure of Geodynamics, 2007. URL: geodynamics.org/cig/software/cs/cigma/cigma.pdf

CIG requests that in your oral presentations and in your papers that you indicate your use of this code and acknowledge the author of the code and CIG (`geodynamics.org`).

1.3 Support

Cigma development is supported by a grant from the National Science Foundation to CIG, managed by the California Institute of Technology.

Chapter 2

Installation and Getting Help

2.1 Getting Help

For help, send an e-mail to the CIG Computational Science Mailing List (`cig-cs@geodynamics.org`). You can subscribe to the `cig-cs` mailing list and view archived discussions at the CIG Mail Lists web page (`geodynamics.org/cig/lists`). If you encounter any bugs or have problems installing Cigma, please submit a report to the CIG Bug Tracker (`geodynamics.org/bugs`).

2.2 Installation from Source

To use Cigma, download the source package (in the form of a compressed tar file) from the CIG Cigma web page (`geodynamics.org/cig/software/packages/cs/cigma`). This step will require the GNU C and C++ compilers. After unpacking the source and installing the dependencies, issue the following commands

```
$ make
$ sudo make install
```

2.2.1 HDF5

HDF5 is available for download from The HDF Group (`hdfgroup.org/HDF5`). Binaries can be obtained at hdfgroup.org/HDF5/release/obtain5.html (`hdfgroup.org/HDF5/release/obtain5.html`). To install from source, download the latest stable version of this library (currently 1.6.5) and issue the following commands

```
$ tar xvfz hdf5-1.6.5
$ cd hdf5-1.6.5
$ ./configure
$ make
$ sudo make install
```

2.2.2 PyTables

PyTables is a Python extension module that builds on top of the HDF5 library. It provides a convenient scripting interface to manipulate HDF5 files. It is available from PyTables (`www.pytables.org`).

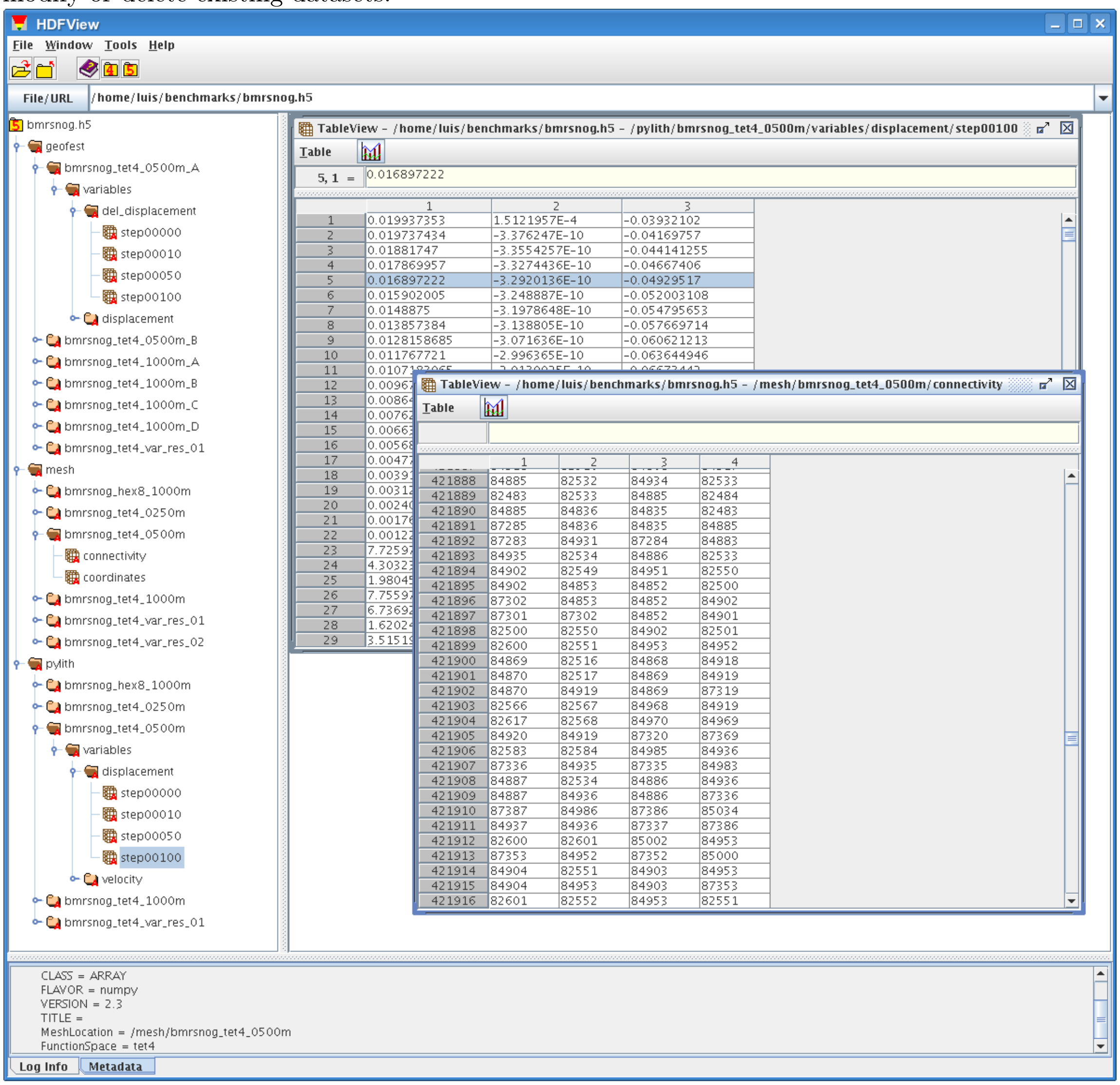
To install this extension from source, download the latest stable version (currently 2.0) and issue the following commands

```
$ tar xvfz pytables-2.0
$ cd pytables-2.0
$ sudo python setup.py install
```

2.2.3 HDFView (optional)

NCSA HDFView is a graphical user interface tool for accessing data in your HDF5 files. You can use it for viewing the internal file hierarchy in a tree structure, adding new datasets, and modifying or deleting existing datasets. You can download it from the HDFView home page (`hdf.ncsa.uiuc.edu/hdf-java-html/hdfview`).

Figure 2.1: With HFDFView, you can view the internal file hierarchy in a tree structure, add new datasets, and modify or delete existing datasets.



Chapter 3

Error Analysis

3.1 Introduction

When studying differential equations that represent physical systems we often obtain solutions by using a variety of techniques, most of which are numerical in nature. In carefully designed problems one may of course obtain solutions in explicit analytical form, but for the most part we will deal with approximate solutions given by the Finite Element Method. Without any closed-form solution available, the quality of an approximation can only be assessed relative to other approximations.

Thus, an important part of error analysis lies in the ability to calculate the distance between two putative solutions. Estimating the error between two arbitrarily represented fields is computationally challenging due to the variety of representations that are possible. For example, each field may use its own discretization of the original domain, and may use a different set of shape functions.

3.2 Distance Measures

The simplest possible quantitative measure of the difference between two distinct fields you can make consists of taking the pointwise difference of both fields at a common set of points. While no finite sample of points can perfectly represent a continuum of values, valuable information can be inferred from a statistics analysis of the resulting residual values.

Another useful distance measure can be obtained by using the L_2 norm, defined by the following integral

$$\varepsilon = ||u - v||_{L_2} = \sqrt{\int_\Omega ||u(\vec{x}) - v(\vec{x})||^2 d\vec{x}}$$

This gives us a single global estimate ε representing the distance between the two fields $u(\vec{x})$ and $v(\vec{x})$. Alternatively, you may think of this as the size, or norm, of the residual field $\rho(\vec{x}) = u(\vec{x}) - v(\vec{x})$. If we discretize the domain Ω into finite elements Ω_e, the above integral can be broken up into a sum over local contributions on each element. For efficiency, each contribution can be integrated over a reference element $\hat{\Omega}_e$ defined on a standard coordinate system.

$$\begin{aligned}
\varepsilon^2 &= \sum_{e=1}^{\text{nel}} \varepsilon_e^2 \\
&= \sum_{e=1}^{\text{nel}} \int_{\Omega_e} ||u(\vec{x}) - v(\vec{x})||^2 d\vec{x} \\
&= \sum_{e=1}^{\text{nel}} \int_{\hat{\Omega}_e} ||u(\vec{\xi}) - v(\vec{\xi})||^2 J(\vec{\xi}) d\vec{\xi}
\end{aligned}$$

In general, we won't be able to integrate each local contribution exactly since the two fields u and v may have a representation that's incompatible with the local domain Ω_e. However, we can approximate each ε_e^2 by applying an appropriate quadrature rule with a tolerable truncation error [2].

Assuming we apply the same quadrature rule, with weights w_q and integration points $\vec{\xi}_q$, on every element,

$$\begin{aligned} \varepsilon_e^2 &= \sum_{q=1}^{\mathrm{nq}} w_q ||\hat{\rho}(\vec{x}_q)||^2 \\ &= \sum_{q=1}^{\mathrm{nq}} w_q ||u(\vec{\xi}_q) - v(\vec{\xi}_q)||^2 J(\vec{\xi}_q) \end{aligned}$$

thus we arrive at the final form

$$\varepsilon = \sqrt{\sum_{e=1}^{\mathrm{nel}} \sum_{q=1}^{\mathrm{nq}} w_q ||u(\vec{\xi}_q) - v(\vec{\xi}_q)||^2 J(\vec{\xi}_q)}$$

In calculating the norm of the residual field ρ, Cigma will output each of the local contributions ε_e^2 which by definition are scalar-valued cell quantities over each of their corresponding elements Ω_e.

Chapter 4

Cigma Components

4.1 Mesh

In Cigma, we define a finite element mesh simply by the coordinates, (x_n, y_n, z_n) of its degrees of freedom, and the connectivity relations $\Omega_e = \{n_1, n_2, \ldots\}$ among them which define each individual element in the corresponding discretization.

4.2 Fields

A field is a function which assigns a physical quantity to every point in space. This quantity may correspond to a scalar, a vector, or even a tensor. For any given differential equation problem, a finite element approximation to an unknown field $\phi(\vec{x})$ as a weighed sum over a fixed set of localized shape functions $\phi_n(\vec{x})$.

$$\phi(\vec{x}) = \sum_{n=1}^{N} d_n \phi_n(\vec{x})$$

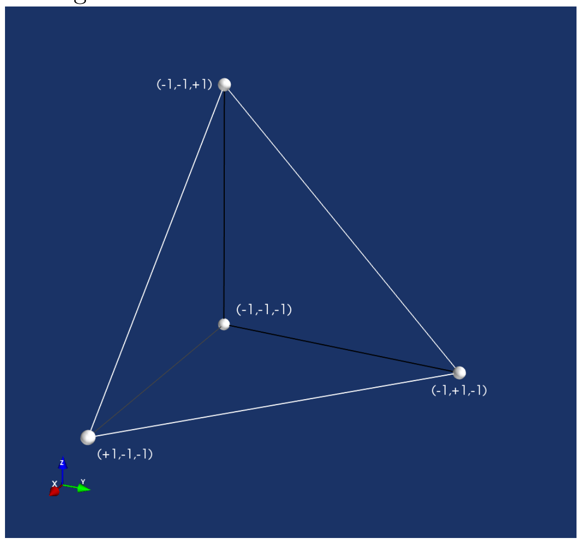
Naturally, once the weights d_n, or degrees of freedom as they are also called, are known to us, we can evaluate $\phi(\vec{x})$ at any point $\vec{x}$ we desire. Thus, in Cigma a field is represented simply by a list of degrees of freedom d_n, which may be a scalar, vector or tensor quantity, depending on the nature of ϕ.

4.3 Elements

This release of Cigma provides you with two built-in finite element spaces shown below. The location of each element is indexed into a spatial database in order to speed up the evaluation process.

Function Space tet4

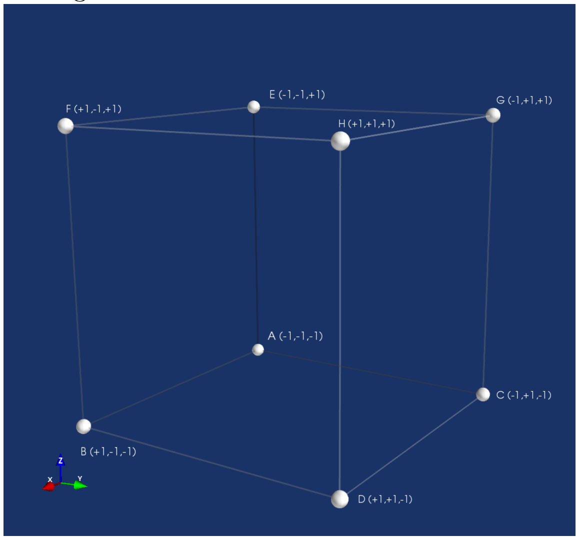
Figure 4.1: Reference tetrahedral element



$$
\begin{aligned}
TN_a &= \frac{1}{2}(-1 - x - y - z) \\
TN_b &= \frac{1}{2}(1 + x) \\
TN_c &= \frac{1}{2}(1 + y) \\
TN_d &= \frac{1}{2}(1 + z)
\end{aligned}
$$

Function Space hex8

Figure 4.2: Reference hexahedral element



$$
\begin{aligned}
HN_a &= \frac{1}{8}(1-x)(1-y)(1-z) \\
HN_b &= \frac{1}{8}(1+x)(1-y)(1-z) \\
HN_c &= \frac{1}{8}(1-x)(1+y)(1-z) \\
HN_d &= \frac{1}{8}(1+x)(1+y)(1-z) \\
HN_e &= \frac{1}{8}(1-x)(1-y)(1+z) \\
HN_f &= \frac{1}{8}(1+x)(1-y)(1+z) \\
HN_g &= \frac{1}{8}(1-x)(1+y)(1+z) \\
HN_h &= \frac{1}{8}(1+x)(1+y)(1+z)
\end{aligned}
$$

Chapter 5

Running Cigma

5.1 Comparing Two Fields

Comparing two arbitrary finite element fields can be accomplished with the `cigma-compare` command line utility, which takes a number of arguments in order to facilitate writing shell scripts. The comparisons always take place using the mesh of the first field. Note that the first and second arguments take the special form `filename:dataset`. Finally, the square of each of the local residual values are written to the specified VTK output file as cell-based scalars.

To use a quadrature rule for the field comparisons, you can specify arguments similar to the following

```
cigma-compare --output=squared-residuals.vtk   \
              --first=field1.h5:/field1/stepN  \
              --second=field2.h5:/field2/stepN \
              --rule=qr.h5:/path/to/rule
```

Alternatively, to perform a pointwise comparison at random sample points inside each element in the first mesh, you can use arguments similar to the following

```
cigma-compare --output=squared-residuals.vtk   \
              --first=field1.h5:/field1/stepN  \
              --second=field2.h5:/field2/stepN \
              --samples-per-element=1
```

5.2 Input Format

The Hierarchical Data Format (HDF) is a portable file format developed at the National Center for Supercomputing Applications (NCSA) (`hdf.ncsa.uiuc.edu/HDF5`). It is designed for storing, retrieving, analyzing, visualizing, and converting scientific data. The current and most popular version is HDF5, which stores multi-dimensional arrays together with ancillary data in a portable self-describing format. It uses a hierarchical structure that provides application programmers with a host of options for organizing how data is stored in HDF5 files.

HDF5 files are organized in a hierarchical structure, similar to a UNIX file system. Two types of primary objects, groups and datasets, are stored in this structure. A group contains instances of zero or more groups or datasets, while a dataset stores a multi-dimensional array of data elements. Both kinds of objects are accompanied by supporting metadata.

A dataset is physically stored in two parts: a header and a data array. The header contains miscellaneous metadata describing the dataset as well as information that is needed to interpret the array portion of the dataset. Essentially, it includes the name, datatype, dataspace, and storage layout of the dataset. The name is a text string identifying the dataset. The datatype describes the type of the data array elements. The dataspace defines the dimensionality of the dataset, i.e., the size and shape of the multi-dimensional array.

Using HDF5 datasets in Cigma allows us to avoid having to convert between too many distinct formats. Moreover, due to the amount of disk I/O, large finite element meshes can be handled more efficiently in binary format. A typical Cigma HDF5 file has the following structure:

```
model.h5
\__ model
    |__ mesh
    |   |__ coordinates    [nno x nsd]
    |   \__ connectivity   [nel x ndof]
    \__ variables
        \__ velocity
            \__ step00010  [nno x ndim]
```

You have a certain amount of flexibility in grouping your own data. Cigma will only require you to provide a small amount of metadata on your field and mesh datasets, described below:

MeshID a universally unique identifier (uuid) assigned to the mesh for easily distinguishing identical meshes.

MeshLocation points to the HDF5 group which contains the appropriate coordinates and connectivity datasets.

FunctionSpace string identifier to determine which shape functions to use for interpolating values inside the element.

5.2.1 Importing Data

In its source distribution, Cigma provides two examples for importing data from two different codes into its standard HDF5 format.

Mesh coordinates can be specified in the following format

```
nno nsd
1 x1 y1 z1
2 x2 y2 z2
3 x3 y3 z3
...
```

Mesh connectivity with

```
nel ndof
1 node_1 node_2 node_3 node_4 ...
2 node_1 node_2 node_3 node_4 ...
3 node_1 node_2 node_3 node_4 ...
...
```

A generic field with `ndim` components is specified by

```
nno ndim
1 f1 f2 f3 ..
2 f1 f2 f3 ..
...
```

Chapter 6

Visualization

As can be seen from the two images in Figure 6.1, simply visualizing two different solutions side by side does not give you enough insight into their actual differences. By using Cigma to calculate the residual field between them, you can get a better idea for how the local contributions to the global error are distributed both spatially and temporally.

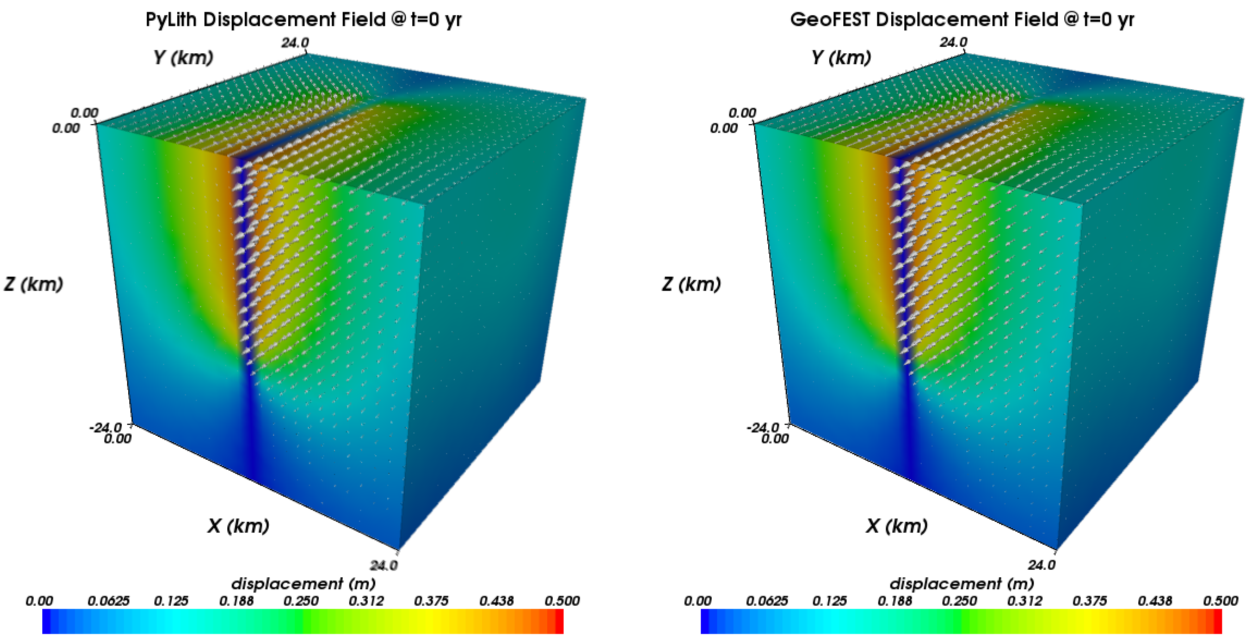


Figure 6.1: Solution of a viscoelastic problem with a fault using two finite element codes: PyLith solution (left) and GeoFEST solution (right).

6.1 Benchmark Cases

Here we compare the output from two codes, PyLith-0.8 and GeoFEST-4.5, on two benchmark cases (`geodynamics.org/cig/workinggroups/short/workarea/benchmarks`) defined by the CIG Short-Term Tectonics working group. They are both defined on cube domain (Figure 6.2) with sides having a length of 24 km, consisting of two layers of different material types. The top layer is nearly elastic while the bottom layer follows viscoelastic relaxation of stresses. Bottom and side displacements are set to the elastic analytic solution. A symmetric boundary condition is also imposed on the y=0 plane.

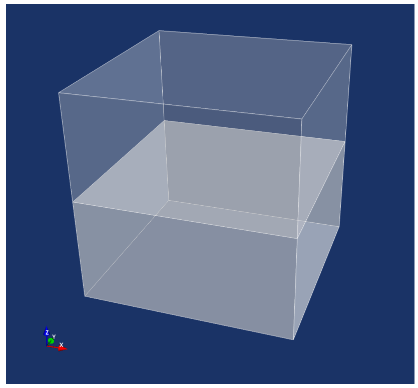


Figure 6.2: Cube domain of 24 km length consisting of two layers of different material types.

The first benchmark problem (left) consists of a vertical right-lateral strike-slip fault. The second benchmark problem consists of a 45-degree dipping reverse fault.

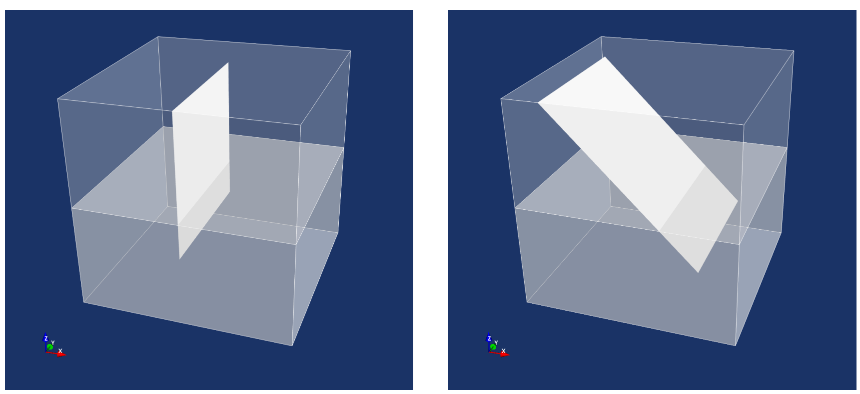


Figure 6.3: Two benchmark problems: (left) Benchmark problem consisting of a vertical right-lateral strike-slip fault; (right) Benchmark problem consisting of a 45-degree dipping reverse fault.

In both cases we solve for the displacement and vector fields at various time steps, namely 0, 1, 5, and 10 years. In the plots below, we show the distribution of the squared local residuals on each cell.

6.1.1 Strike-Slip with No Gravity

In this section, we show ten equally spaced isosurfaces of the displacement field residuals for the strike-slip benchmark (0 and 10 years shown). In Figure 6.1, we see that the differences are very localized at t=0 years. There is not much difference between time steps at t=1, 5 and 10 years, so we are only showing the last time step. Note that the maximum errors are localized to the interface between the two layers on the symmetric boundary.

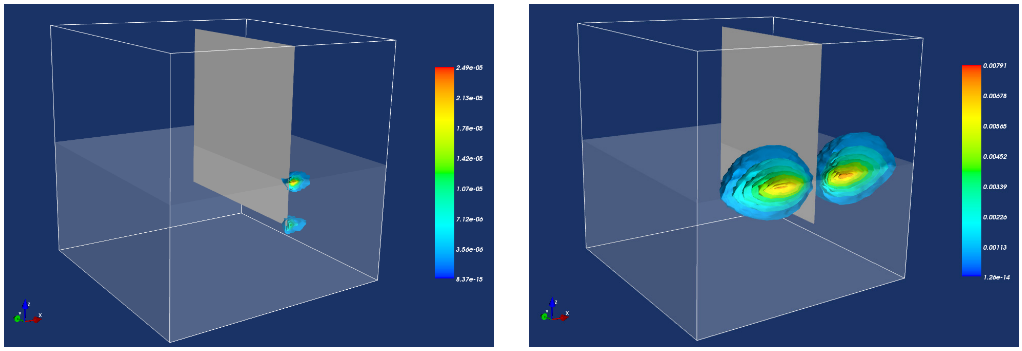


Figure 6.4: Strike-slip: PyLith-GeoFEST comparison of displacement residuals on a 500m resolution mesh (left: t=0 years, right: t=10 years).

Slightly different behavior can be observed in the velocity field residuals. Shown here are ten equally spaced isosurfaces at each time step, where each isosurface is displayed as a point distribution to reveal the inner structure. Note that after 10 years, most of the disagreement occurs inside the bottom viscoelastic layer, centered around the fault's interior sharp corner.

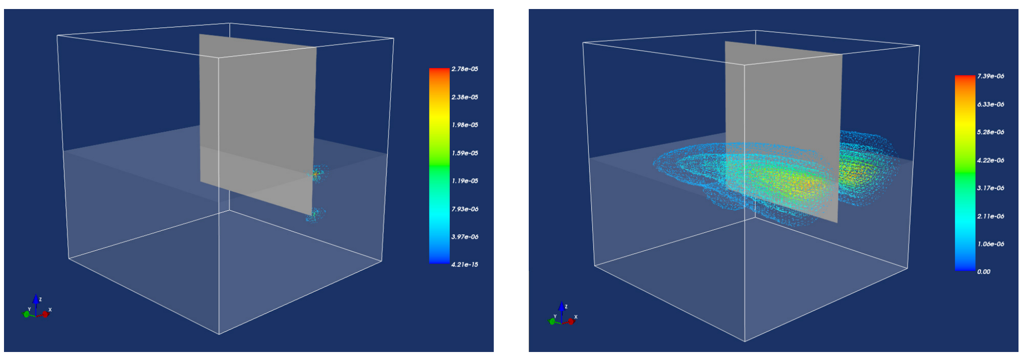


Figure 6.5: Strike-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=0 years, right: t=1 year).

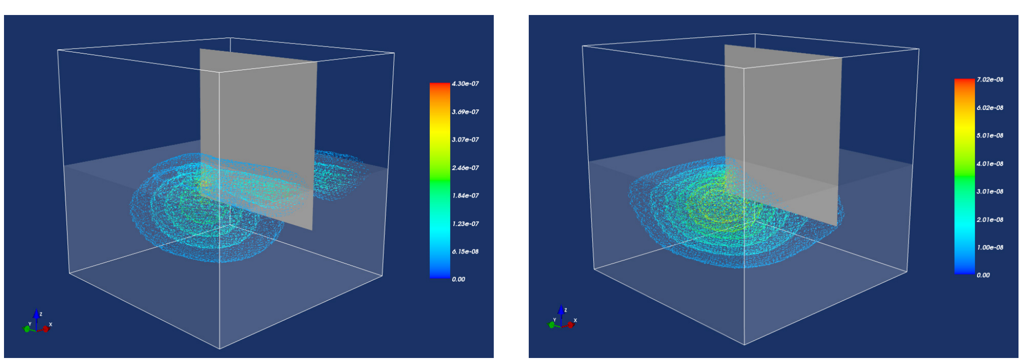


Figure 6.6: Strike-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=5 years, right: t=10 years).

Finally, here is a higher resolution comparison of the displacement residuals at t=0 years, sampled over a 250m resolution mesh. Displayed here are ten equally spaced isosurfaces, nine of which are very near the fault. In this case, the linear taper over the internal edges of the fault is clearly visible.

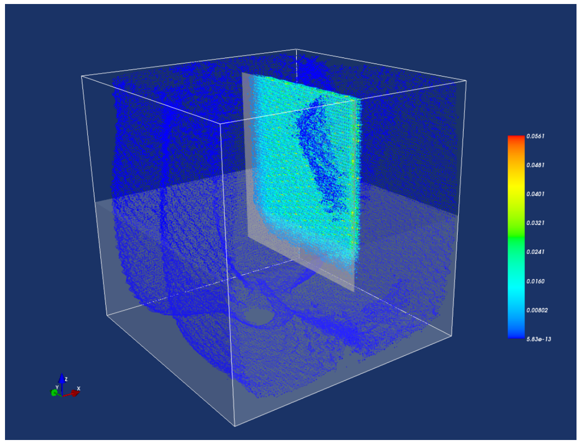


Figure 6.7: Strike-slip: PyLith-GeoFEST comparison of displacement residuals on a 250m resolution mesh (t=0 years).

6.1.2 Reverse-Slip with No Gravity

You can also visualize the distribution of errors by plotting the residual field values over the surface of each cell and applying a threshold filter which eliminates cells containing values outside a threshold interval. Here we show how velocity field residuals in the reverse-slip benchmark are distributed temporally by throwing away all squared residuals lower than $10^{-7}(\mathrm{m/s})^2$

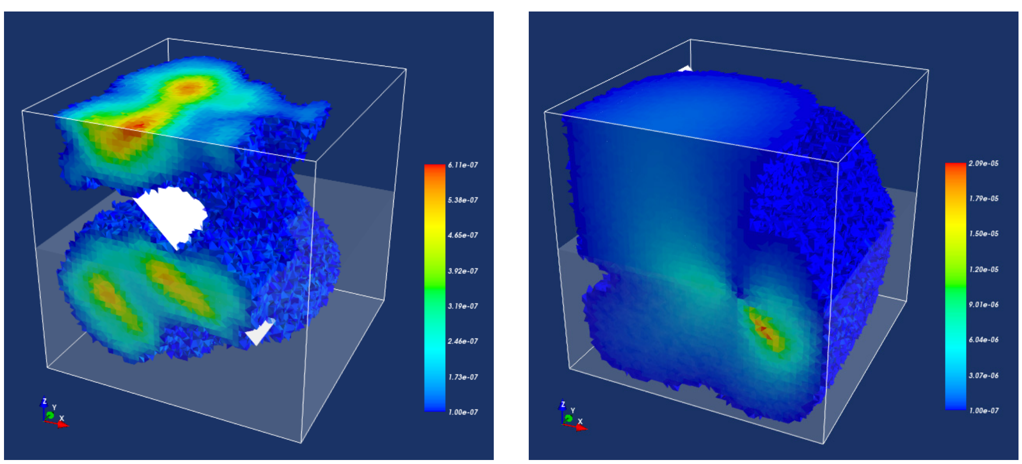


Figure 6.8: Reverse-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=0 years, right: t=1 year).

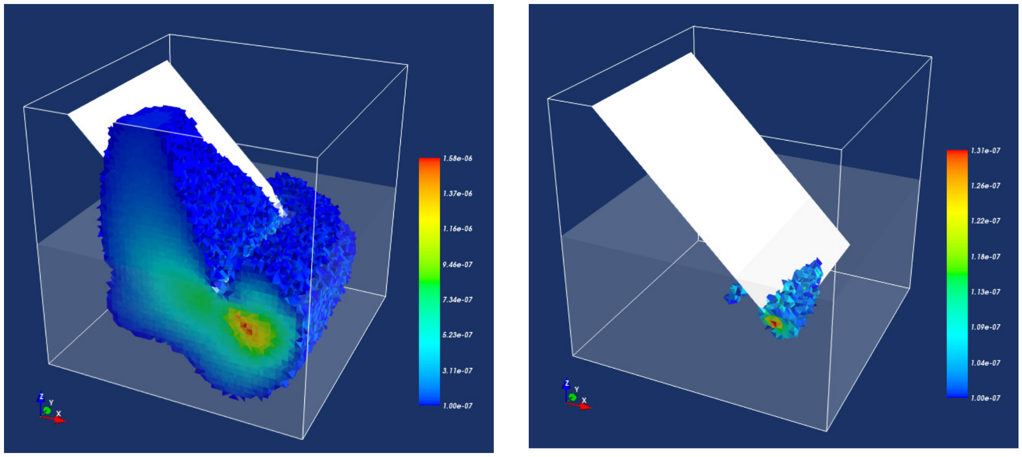


Figure 6.9: Reverse-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=5 years, right: t=10 years).

Finally, below we display ten equally spaced isosurfaces over the displacement field residuals of the reverse-slip benchmark. Note that after 1 year, most of the disagreement occurs in the bottom viscoelastic layer.

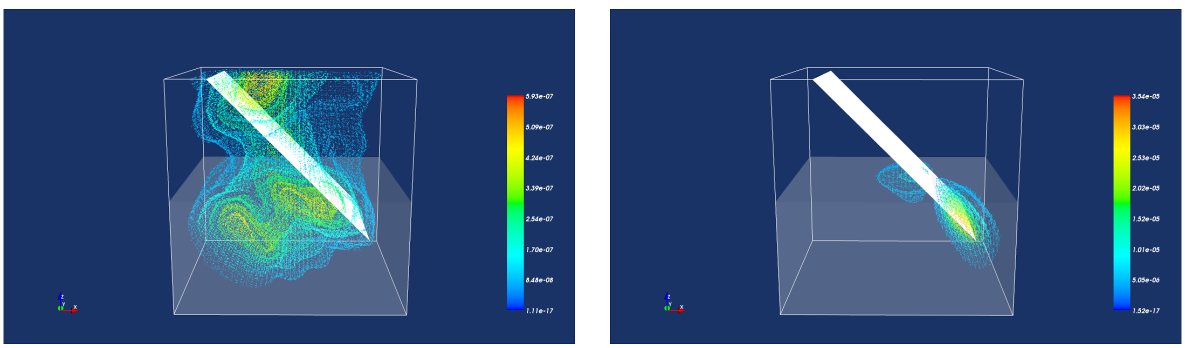


Figure 6.10: Reverse-slip: PyLith-GeoFEST comparison of displacement residuals on a 500m resolution mesh (left: t=0 years, right: t=1 year).

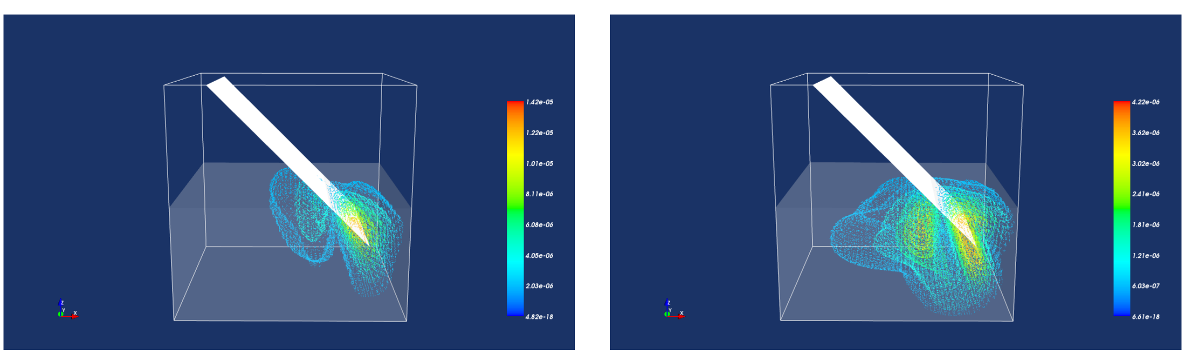
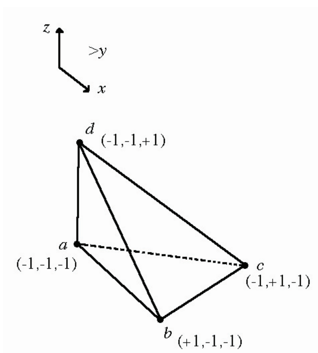


Figure 6.11: Reverse-slip: PyLith-GeoFEST comparison of displacement residuals on a 500m resolution mesh (left: t=5 years, right: t=10 years).

Appendix A

Shape Functions

A.1 Linear Tetrahedral Element (tet4)



$$
\begin{array}{cccccc}
 & & & & \phi & \\
(-1, & -1, & -1) & \mapsto & a \\
(+1, & -1, & -1) & \mapsto & b \\
(-1, & +1, & -1) & \mapsto & c \\
(-1, & -1, & +1) & \mapsto & d
\end{array}
$$

A field $\vec{\varphi} = \varphi_x\hat{x} + \varphi_y\hat{y} + \varphi_z\hat{z}$ defined over a linear tetrahedral element with vertices at $A(x_0, y_0, z_0)$, $B(x_1, y_1, z_1)$, $C(x_2, y_2, z_2)$, $D(x_3, y_3, z_3)$, has the following functional form inside the reference tetrahedral element shown in Figure 6.2.

$$
\begin{aligned}
\varphi_x(\vec{\xi}) &= \alpha_0 + \alpha_1\xi + \alpha_2\eta + \alpha_3\zeta \\
\varphi_y(\vec{\xi}) &= \beta_0 + \beta_1\xi + \beta_2\eta + \beta_3\zeta \\
\varphi_z(\vec{\xi}) &= \gamma_0 + \gamma_1\xi + \gamma_2\eta + \gamma_3\zeta
\end{aligned}
$$

In particular, the map from the reference coordinates into the regular coordinates vector $\vec{x}(\vec{\xi}) = x(\hat{\vec{\xi}})x + y(\vec{\xi})\hat{y} + y(\vec{\xi})\hat{z}$ looks like

$$
\begin{aligned}
x(\vec{\xi}) &= \alpha_0 + \alpha_1\xi + \alpha_2\eta + \alpha_3\zeta \\
y(\vec{\xi}) &= \beta_0 + \beta_1\xi + \beta_2\eta + \beta_3\zeta \\
z(\vec{\xi}) &= \gamma_0 + \gamma_1\xi + \gamma_2\eta + \gamma_3\zeta
\end{aligned}
$$

The following natural mappings uniquely determine the coefficients α_k, β_k, γ_k

$$
\begin{array}{lcl}
\vec{x}(-1,-1,-1) & \mapsto & (x_0, y_0, z_0) \\
\vec{x}(+1,-1,-1) & \mapsto & (x_1, y_1, z_1) \\
\vec{x}(-1,+1,-1) & \mapsto & (x_2, y_2, z_2) \\
\vec{x}(-1,-1,+1) & \mapsto & (x_3, y_3, z_3)
\end{array}
$$

Considering only the first component $x(\vec{\xi})$, we can obtain the matrix equation

$$\begin{array}{c} a \\ b \\ c \\ d \end{array} \begin{bmatrix} 1 & (-1) & (-1) & (-1) \\ 1 & (+1) & (-1) & (-1) \\ 1 & (-1) & (+1) & (-1) \\ 1 & (-1) & (-1) & (+1) \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Applying our desired map to the other two functions yields two other identical systems. Thus we may augment the system as follows,

$$\begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & +1 & -1 & -1 \\ 1 & -1 & +1 & -1 \\ 1 & -1 & -1 & +1 \end{bmatrix} \begin{bmatrix} \alpha_0 & \beta_0 & \gamma_0 \\ \alpha_1 & \beta_1 & \gamma_1 \\ \alpha_2 & \beta_2 & \gamma_2 \\ \alpha_3 & \beta_3 & \gamma_3 \end{bmatrix} = \begin{bmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{bmatrix}$$

Now we can easily invert the square matrix on the left, yielding the values of the unknown coefficients,

$$\begin{bmatrix} \alpha_0 & \beta_0 & \gamma_0 \\ \alpha_1 & \beta_1 & \gamma_1 \\ \alpha_2 & \beta_2 & \gamma_2 \\ \alpha_3 & \beta_3 & \gamma_3 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -1 & 1 & 1 & 1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{bmatrix}$$

Using the values forα_k, we find that $x(\vec{\xi})$ becomes

$$\begin{aligned} x(\vec{\xi}) &= \alpha_0 + \alpha_1\xi + \alpha_2\eta + \alpha_3\zeta \\ &= \left[\frac{1}{2}(-x_0 + x_1 + x_2 + x_3)\right] \\ &\quad + \left[\frac{1}{2}(-x_0 + x_1)\right]\xi \\ &\quad + \left[\frac{1}{2}(-x_0 + x_2)\right]\eta \end{aligned}$$

Rearranging terms, we get

$$\begin{aligned} x(\vec{\xi}) &= \left[\frac{1}{2}(-1 - \xi - \eta - \zeta)\right] x_0 \\ &\quad + \left[\frac{1}{2}(1 + \xi)\right] x_1 \\ &\quad + \left[\frac{1}{2}(1 + \eta)\right] x_2 \\ &\quad + \left[\frac{1}{2}(1 + \zeta)\right] x_3 \end{aligned}$$

$$\begin{aligned} x(\vec{\xi}) &= N_0(\vec{\xi})x_0 + N_1(\vec{\xi})x_1 + N_2(\vec{\xi})x_2 + N_3(\vec{\xi})x_3 \\ y(\vec{\xi}) &= N_0(\vec{\xi})y_0 + N_1(\vec{\xi})y_1 + N_2(\vec{\xi})y_2 + N_3(\vec{\xi})y_3 \\ z(\vec{\xi}) &= N_0(\vec{\xi})z_0 + N_1(\vec{\xi})z_1 + N_2(\vec{\xi})z_2 + N_3(\vec{\xi})z_3 \end{aligned}$$

where

$$
\begin{aligned}
N_0(\vec{\xi}) &= \frac{1}{2}(-1-\xi-\eta-\zeta) \\
N_1(\vec{\xi}) &= \frac{1}{2}(1+\xi) \\
N_2(\vec{\xi}) &= \frac{1}{2}(1+\eta) \\
N_3(\vec{\xi}) &= \frac{1}{2}(1+\zeta)
\end{aligned}
$$

As a final note, observe that we can streamline the evaluation process over any number of points, $\vec{\xi}_0, \vec{\xi}_1, \vec{\xi}_2, \ldots$, inside the same element via the following matrix multiplication

$$
\begin{bmatrix} x(\vec{\xi}_0) & y(\vec{\xi}_0) & z(\vec{\xi}_0) \\ x(\vec{\xi}_1) & y(\vec{\xi}_1) & z(\vec{\xi}_1) \\ x(\vec{\xi}_2) & y(\vec{\xi}_2) & z(\vec{\xi}_2) \\ \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} N_0(\vec{\xi}_0) & N_1(\vec{\xi}_0) & N_2(\vec{\xi}_0) & N_3(\vec{\xi}_0) \\ N_0(\vec{\xi}_1) & N_1(\vec{\xi}_1) & N_2(\vec{\xi}_1) & N_3(\vec{\xi}_1) \\ N_0(\vec{\xi}_2) & N_1(\vec{\xi}_2) & N_2(\vec{\xi}_2) & N_3(\vec{\xi}_2) \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \begin{bmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{bmatrix}
$$

A.1.1 Jacobian Matrix

Recall the definition of the Jacobian matrix:

$$
\frac{\partial \vec{x}}{\partial \vec{\xi}} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \qquad \begin{aligned} x\left(\vec{\xi}\right) &= \textstyle\sum_i N_i\left(\vec{\xi}\right) x_i \\ y\left(\vec{\xi}\right) &= \textstyle\sum_i N_i\left(\vec{\xi}\right) y_i \\ z\left(\vec{\xi}\right) &= \textstyle\sum_i N_i\left(\vec{\xi}\right) z_i \end{aligned}
$$

$$
\frac{\partial x}{\partial \xi} = \sum_i \frac{\partial N_i}{\partial \xi} x_i \quad , \quad \frac{\partial x}{\partial \eta} = \sum_i \frac{\partial N_i}{\partial \eta} x_i \quad , \quad \frac{\partial x}{\partial \zeta} = \sum_i \frac{\partial N_i}{\partial \zeta} x_i
$$

$$
\frac{\partial y}{\partial \xi} = \sum_i \frac{\partial N_i}{\partial \xi} y_i \quad , \quad \frac{\partial y}{\partial \eta} = \sum_i \frac{\partial N_i}{\partial \eta} y_i \quad , \quad \frac{\partial y}{\partial \zeta} = \sum_i \frac{\partial N_i}{\partial \zeta} y_i
$$

$$
\frac{\partial z}{\partial \xi} = \sum_i \frac{\partial N_i}{\partial \xi} z_i \quad , \quad \frac{\partial z}{\partial \eta} = \sum_i \frac{\partial N_i}{\partial \eta} z_i \quad , \quad \frac{\partial z}{\partial \zeta} = \sum_i \frac{\partial N_i}{\partial \zeta} z_i
$$

Applying these to our shape functions on a tetrahedron, we obtain

i	TN_i	$\partial TN_i/\partial\xi$	$\partial TN_i/\partial\eta$	$\partial TN_i/\partial\zeta$
0	$\frac{1}{2}(-1-\xi-\eta-\zeta)$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
1	$\frac{1}{2}(1+\xi)$	$+\frac{1}{2}$	0	0
2	$\frac{1}{2}(1+\eta)$	0	$+\frac{1}{2}$	0
3	$\frac{1}{2}(1+\zeta)$	0	0	$+\frac{1}{2}$

$$\frac{\partial x}{\partial \xi} = \left(-\frac{1}{2}\right) x_0 + \left(\frac{1}{2}\right) x_1 \ , \ \frac{\partial x}{\partial \eta} = \left(-\frac{1}{2}\right) x_0 + \left(\frac{1}{2}\right) x_2 \ , \ \frac{\partial x}{\partial \zeta} = \left(-\frac{1}{2}\right) x_0 + \left(\frac{1}{2}\right) x_3$$

$$\frac{\partial y}{\partial \xi} = \left(-\frac{1}{2}\right) y_0 + \left(\frac{1}{2}\right) y_1 \ , \ \frac{\partial y}{\partial \eta} = \left(-\frac{1}{2}\right) y_0 + \left(\frac{1}{2}\right) y_2 \ , \ \frac{\partial y}{\partial \zeta} = \left(-\frac{1}{2}\right) y_0 + \left(\frac{1}{2}\right) y_3$$

$$\frac{\partial z}{\partial \xi} = \left(-\frac{1}{2}\right) z_0 + \left(\frac{1}{2}\right) z_1 \ , \ \frac{\partial z}{\partial \eta} = \left(-\frac{1}{2}\right) z_0 + \left(\frac{1}{2}\right) z_2 \ , \ \frac{\partial z}{\partial \zeta} = \left(-\frac{1}{2}\right) z_0 + \left(\frac{1}{2}\right) z_3$$

$$\mathrm{J} = \left|\frac{\partial \vec{x}}{\partial \vec{\xi}}\right| = \begin{vmatrix} \frac{1}{2}(x_1 - x_0) & \frac{1}{2}(x_2 - x_0) & \frac{1}{2}(x_3 - x_0) \\ \frac{1}{2}(y_1 - y_0) & \frac{1}{2}(y_2 - y_0) & \frac{1}{2}(y_3 - y_0) \\ \frac{1}{2}(z_1 - z_0) & \frac{1}{2}(z_2 - z_0) & \frac{1}{2}(z_3 - z_0) \end{vmatrix}$$

$$= \frac{1}{8} \begin{vmatrix} 1 & x_0 & y_0 & z_0 \\ 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \end{vmatrix}$$

Appendix B

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