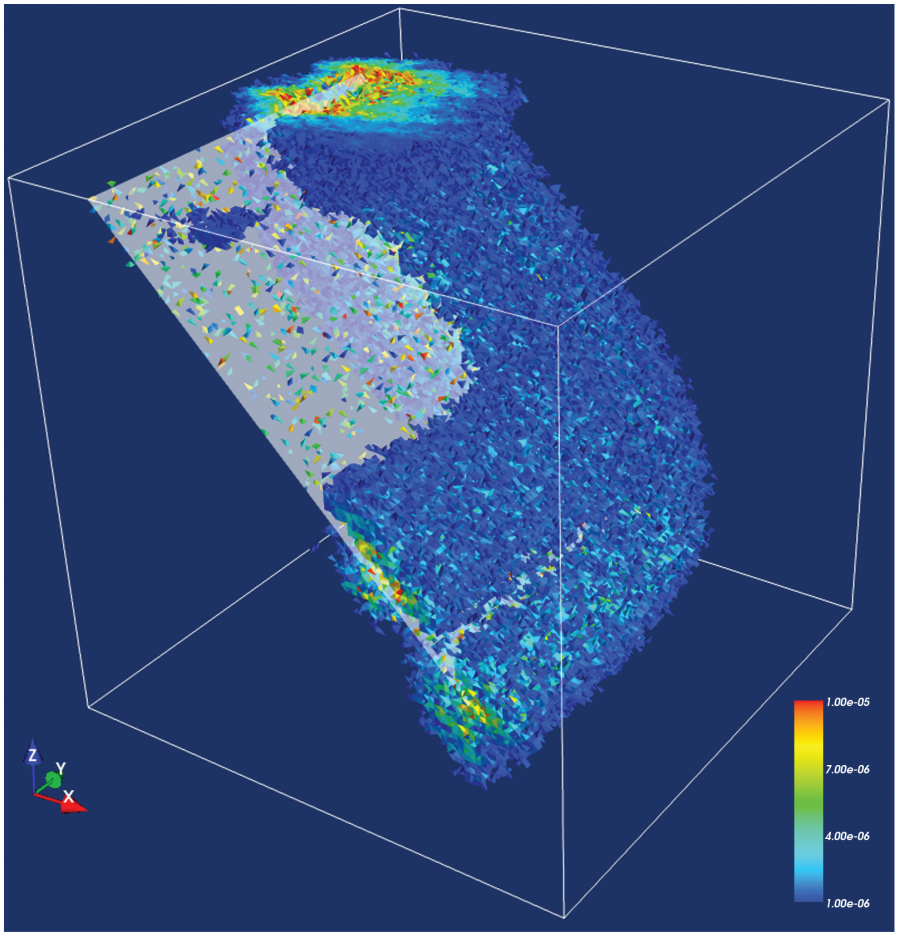
COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)

Cigma

User Manual
Version 0.9.5



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Cigma

Version 0.9.5

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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. The code is being released under the GNU General Public License.

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 Installating 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 VTK

VTK is available from Kitware, Inc. (`www.vtk.org/get-software.php`). If you obtain the binaries from a package manager, make sure to install the associated development headers along with the library. To enable VTK support in Cigma, use the following flags in the configure step:

```
./configure –with-vtk=/path/to/vtk
```

2.2.3 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, which can be used to manipulate the input/output files created by Cigma. PyTables is available for download from PyTables (`www.pytables.org`).

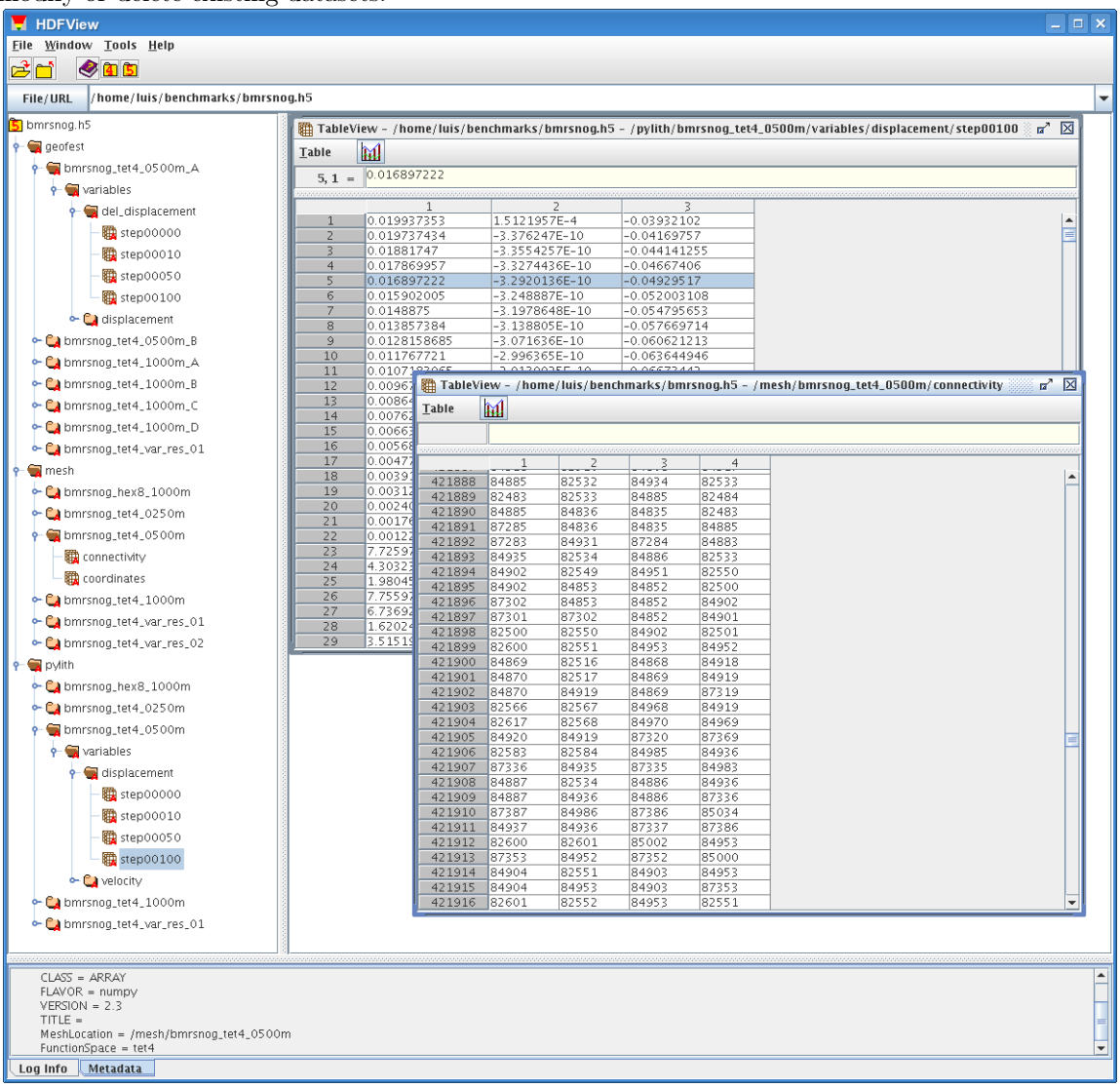
To install this extension from source, download the latest stable version (currently 2.0) and issue the following commands

$ tar xvfz pytables-2.x
$ cd pytables-2.x
$ sudo python setup.py install

2.2.4 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,

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

thus we arrive at the final form

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

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.

Cigma Components

3.3 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.

3.4 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 $\phi_n(\vec{x})$.

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

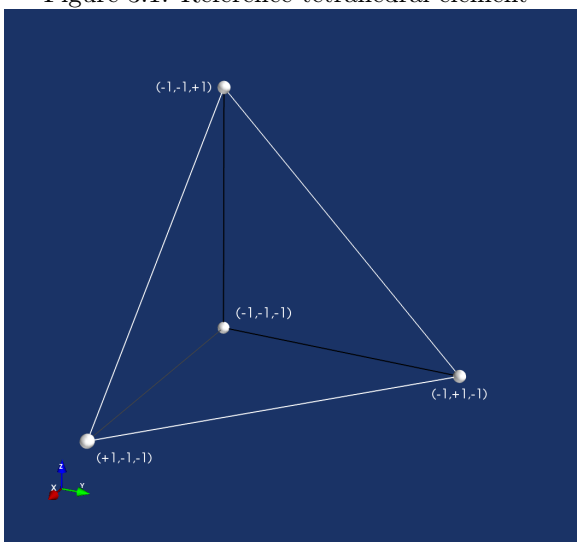
Naturally, once the weights d_n, or degrees of freedom as they are also called, are known to us, we can evaluate $\phi(\vec{x})$ at any point $\vec{x}$ we desire. Thus, in Cigma a field is represented simply by a list of degrees of freedom d_n, which may be a scalar, vector or tensor quantity, depending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

3.5 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

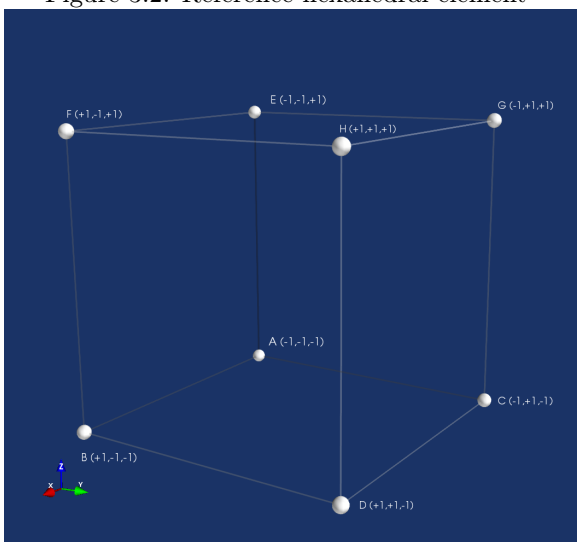
Figure 3.1: Reference tetrahedral element



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

Function Space hex8

Figure 3.2: Reference hexahedral element



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

3.6 Input Formats

The underlying data storage format for Cigma is HDF5, although VTK files can also be specified as input if the VTK development libraries are installed when you configure and compile Cigma. As described in Chapter 4, you can easily examine the structure of an input file by using the `cigma list` command, which will simply reveal the names and dimensions of all datasets inside the specified file.

3.6.1 HDF5

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 known as attributes.

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. Generally, Cigma will only require you to specify the path to a specific field dataset, along with a small amount of metadata on your field and mesh datasets, described below:

MeshID an identifier assigned for use in linking child datasets to their parent mesh.

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 (e.g., tet4, hex8, quad4, tri3, ...).

DatasetType string identifier for classifying the type of data contained in the dataset (e.g., points, connectivity, degrees of freedom, quadrature rules, global quadrature points, global field values).

3.6.2 VTK Files

The Visualization Toolkit (VTK) is a popular open source graphics library for scientific visualizations.

3.6.3 Text Files

Importing and exporting data into simple text can be accomplished with the `cigma copy` command. The format is always in table form, with the dimensions specified in the first line. For example, 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 ndofs
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 (i.e., scalar, vector, or tensor) is specified by

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

In this last case, the number of rows could refer to either `nno` or `nel`, depending on whether the field is node-based or cell-based.

Chapter 4

Running Cigma

Cigma is designed to be scriptable, and thus all operations can be specified as command line arguments given to a single executable called `cigma`. The available commands can be listed with `cigma --help`, and help on a specific command can be obtained with `cigma help <command>`.

Since Cigma is used for obtaining error estimates between arbitrary fields, its primary operation involves the `compare` command. You will need to provide two datasets describing each of the two fields, along with an integration rule and a mesh over which to integrate, although these last two will have reasonable defaults if they are not specified.

Specifying the complete path to a dataset consists of the special form `filepath:dataset`, a colon-delimited pair of file path and dataset path.

4.1 Listing Data

Since Cigma relies so much on being able to specify dataset paths, we have provided a command called `list` for viewing the structure of input file. Its usage is very simple:

To view the structure of an HDF5 file:
$ **cigma list file.h5**
/mesh/coordinates Dataset {119827, 3}
/mesh/connectivity Dataset {661929, 4}
/vars/displacement/step0 Dataset {119827, 3}
/residuals/comparison0 Dataset {661929, 1}
If VTK support is enabled, you can view the structure of a VTK file with:
$ **cigma list file.vtk**
Reading file.vtk
Points = 119827
Cells = 661929
PointDataArray[0] = displacements_t0 (119827 x 3)

4.2 Converting Data

In order to easily move data into and out of the HDF5 format, you can use the `cigma copy` command. By default, it relies on the file extension to detect what format to use when reading or writing data. Various examples are given below.

Usage is typically
cigma copy <source-path> <destination-path>
cigma copy –source=<path> –destination=<path>
cigma copy -s <path> -d <path>

To dump the mesh information into a text file:
cigma copy –source=file.h5:/model/mesh/coords –destination=model-coords.txt
cigma copy –source=file.h5:/model/mesh/connect –destination=model-connect.txt
To import a scalar field `pressure0` from a VTK file into an HDF5 file:
cigma copy –source=file.vtk:pressure0 –destination=file.h5:/model/variables/pressure/t0
To import a vector field called `displacement15` from a VTK file into an HDF5 file:
cigma copy –source=file.vtk:displacement15 –destination=file.h5:/model/variables/displacement/t15
To convert residual data into a VTK file, and then into ASCII:
cigma copy –source=file.h5:/model/residuals/pressure0 –destination=pressure0-residuals.vtk
cigma copy –source=pressure0-residuals.vtk –destination=residuals.txt

4.3 Metadata

As described in a previous chapter on the HDF5 input files, you can attach arbitrary metadata to any number of your datasets or groups. Cigma will make use of a few reserved attributes to determine which mesh and shape functions to use on a particular dataset, but in general you are free to assign your own.

Usage is typically:
cigma set <target-object-path> <attribute-name>[:<type>] <value>
cigma get <target-object-path> [<attribute>]

For example,
cigma set –target=file.h5:/model/ –attribute=AUTHOR –value='John Doe'
cigma set –target=file.h5:/model/vars/pressure –attribute=Units –value=MPa
cigma set –target=file.h5:/model/vars/pressure/t10 –attribute=Step:int32 –value=10
cigma set –target=file.h5:/model/vars/pressure/t10 –attribute=MeshID:int32 –value=1234
cigma set –target=file.h5:/model/vars/pressure/t10 –attribute=FunctionSpace –value=tet4

4.4 Comparing Two Fields

Comparing two arbitrary finite element fields can be accomplished with the `'cigma compare'` command line utility. By default, the comparison will take place over the elements in the mesh of the first field. Finally, the square of each of the local residual values are written to the specified VTK output file as cell-based scalars.

A basic comparison can be as simple as specifying the following arguments:
cigma compare –output=squared-residuals.vtk \
–first=field1.h5:/field1/stepN \
–second=field2.h5:/field2/stepN

4.4.1 Specifying a Mesh

To override the mesh used in the integration, you can specify an extra argument providing the location of the mesh:

cigma compare –mesh=mesh.h5:/model/mesh/ \
[...]

You can also specify the coordinates and connectivity arrays separately, in case they reside in separate files.

cigma compare –mesh-coordinates=file1.h5:/model/mesh/coordinates \
–mesh-connectivity=file2.h5:/model/mesh/connectivity \
[...]

4.4.2 Specifying a Quadrature Rule

If you wish to specify your own quadrature rule, you will have to provide the quadrature weights and points in the appropriate reference element. This can be done with the following additional argument:

**cigma compare –rule=quadrature-rules.h5:/path/to/rule **
[...]

You may also specify the location of the points and weights separately:

**cigma compare –rule-points=file.h5:/path/to/rule/points **
**–rule-weights=file.h5:/path/to/rule/weights **
[...]

Alternatively, to perform a pointwise comparison at random sample points inside each element in the first mesh,

**cigma compare –samples-per-element=1 **
[...]

4.4.3 Against Known Values

A finite element description might not always be available for one of the fields. However, you can break the comparison into several steps if you have a means to compute that field on any of the required points.

First, extract the global coordinates of the integration points. This will result in an explicit list of points over which to evaluate your field.

cigma extract –mesh=field1.h5:/model/mesh/ \
–output=points.h5:/points

At this point, one possibility would be to dump explicit the list of points to a text file, generate the corresponding list of values on your own and import that lsit of values back into an HDF5 file that Cigma can understand.

cigma copy –source=points.h5:/points \
–destination=points.txt
create values.txt
cigma copy –source=values.txt \
–destination=values.h5:/stepN_values

Lastly, you can provide the path to the explicit set of values with

cigma compare –output=squared-residuals.vtk
–first=field1.h5:/field1/stepN
–second=values.h5:/stepN_values

4.4.4 Against a Known Function

If one of your fields is easily described by an analytic expression, then you also have the option to compile your analytic function into cigma, which will enable the `compare` command to reference your function by name:

**cigma compare –output=squared-residuals.vtk **
**–first=field1.h5:/vars/displacement/step0 **
–second=disloc3d

You may also interact with your analytic function by using the `cigma eval` command, and obtain a set of values which may then be passed back to the compare command.

cigma eval –function=disloc3d \
–points=points.h5:/points \
–values=values.h5:/disloc3d_values
cigma compare –output=squared-residuals.vtk \
–first=field1.h5:/vars/displacement/step0 \
–second=values.h5:/disloc3d_values

Chapter 5

Visualization

As can be seen from the two images in Figure 5.1, 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.

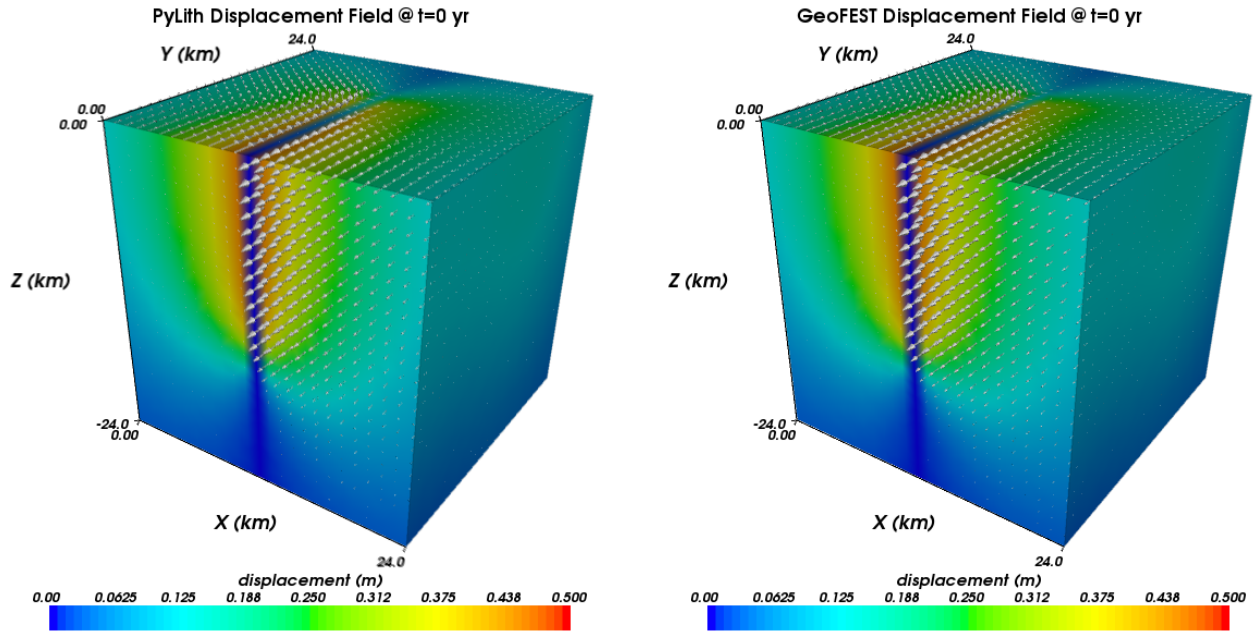


Figure 5.1: Solution of a viscoelastic problem with a fault using two finite element codes: PyLith solution (left) and GeoFEST solution (right).

5.1 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 5.2) 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.

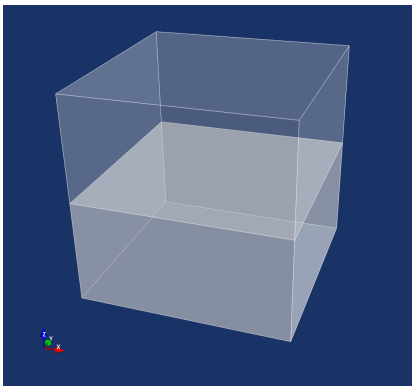


Figure 5.2: Cube domain of 24 km length consisting of two layers of different material types.

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.

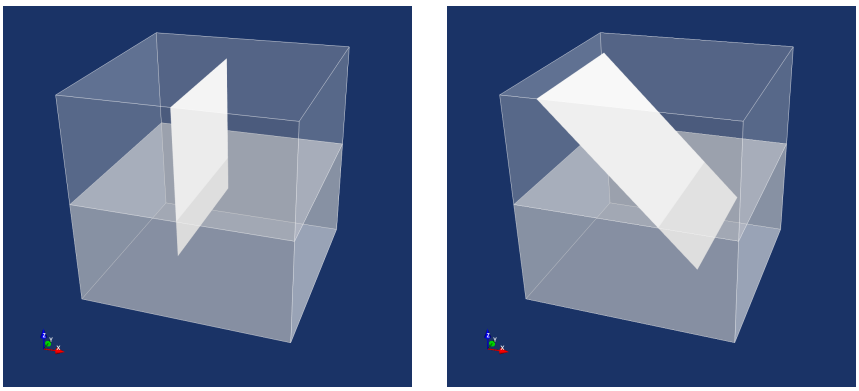


Figure 5.3: Two benchmark problems: (left) Benchmark problem consisting of a vertical right-lateral strike-slip fault; (right) Benchmark problem consisting of a 45-degree dipping reverse fault.

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.

5.1.1 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 5.1, 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.

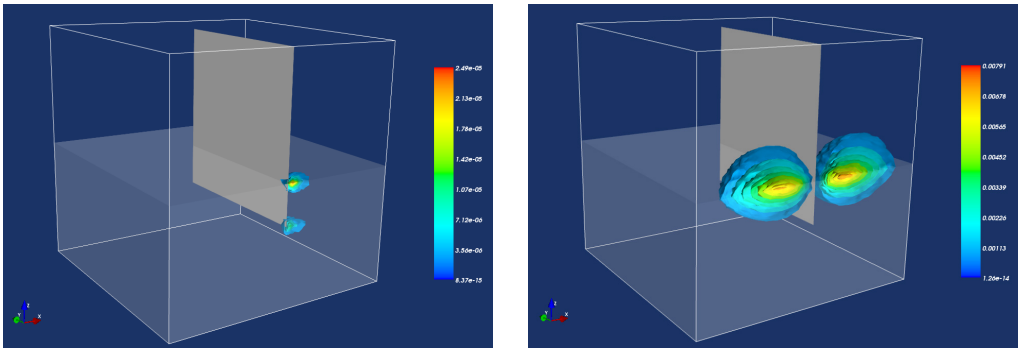


Figure 5.4: Strike-slip: PyLith-GeoFEST comparison of displacement residuals on a 500m resolution mesh (left: t=0 years, right: t=10 years).

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.

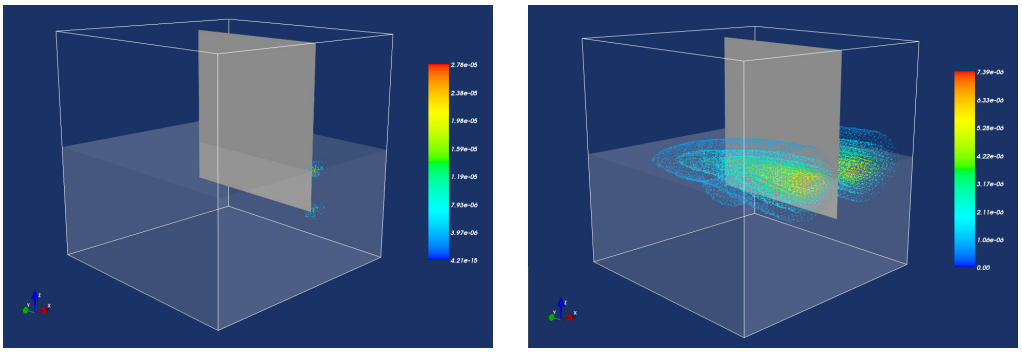


Figure 5.5: Strike-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=0 years, right: t=1 year).

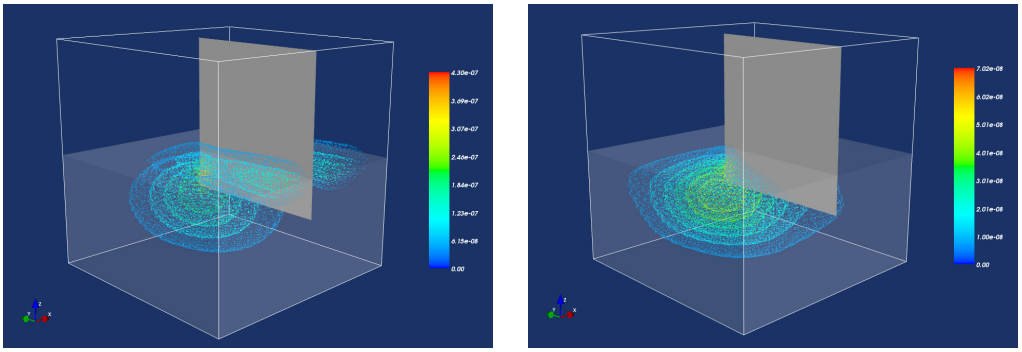


Figure 5.6: Strike-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=5 years, right: t=10 years).

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.

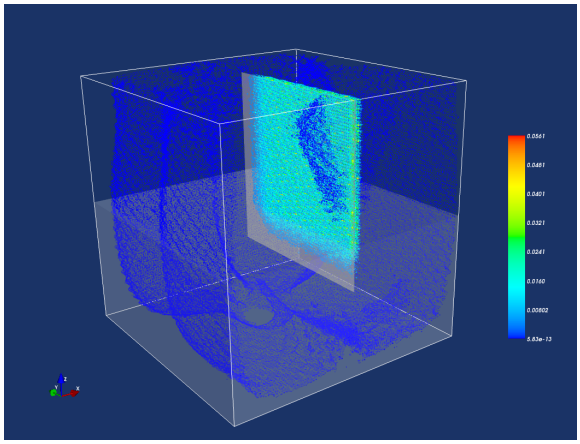


Figure 5.7: Strike-slip: PyLith-GeoFEST comparison of displacement residuals on a 250m resolution mesh (t=0 years).

5.1.2 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 $10^{-7}(\mathrm{m/s})^2$

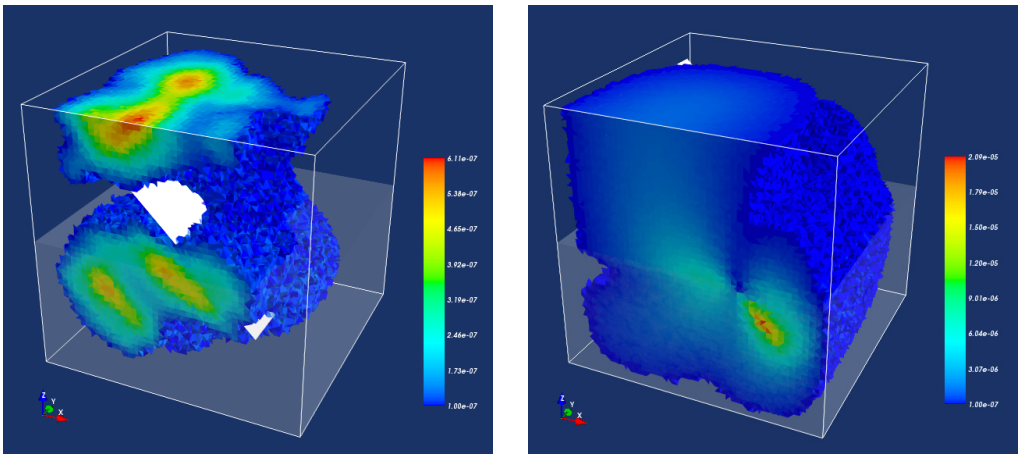


Figure 5.8: Reverse-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=0 years, right: t=1 year).

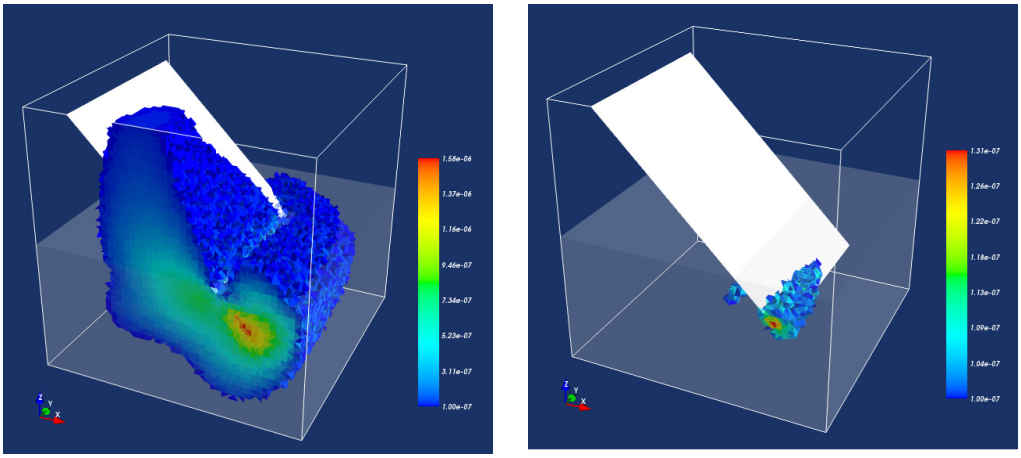


Figure 5.9: Reverse-slip: PyLith-GeoFEST comparison of velocity residuals on a 500m resolution mesh (left: t=5 years, right: t=10 years).

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.

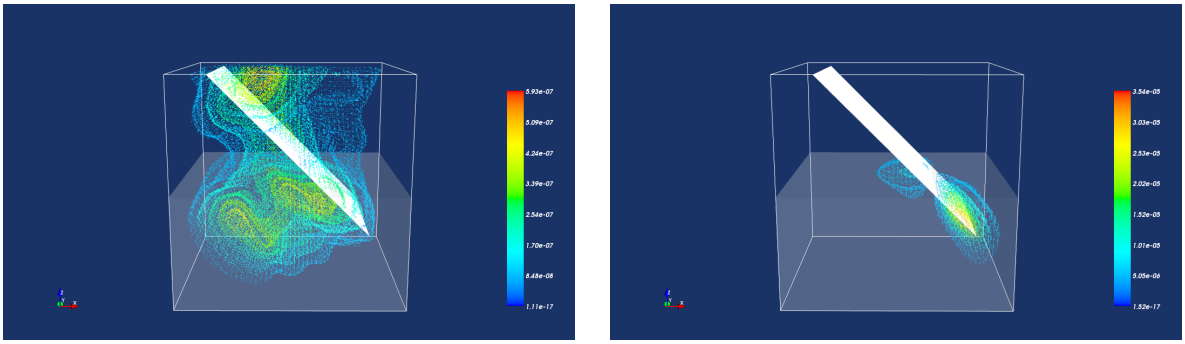


Figure 5.10: Reverse-slip: PyLith-GeoFEST comparison of displacement residuals on a 500m resolution mesh (left: t=0 years, right: t=1 year).

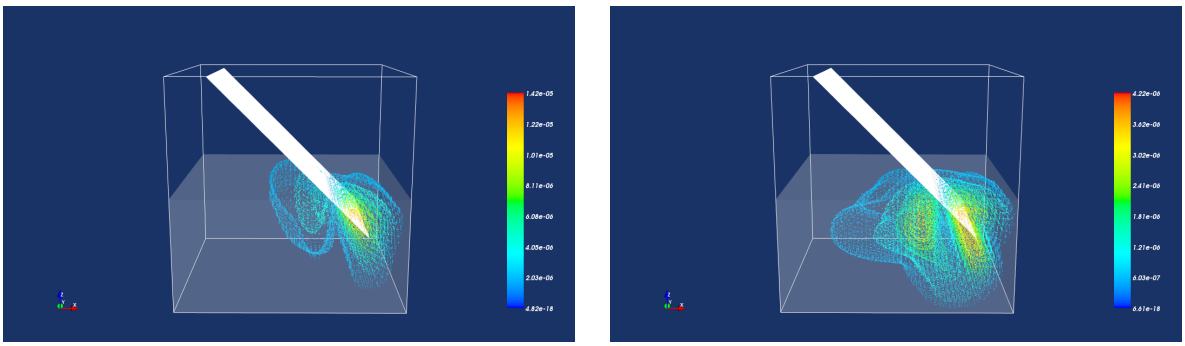
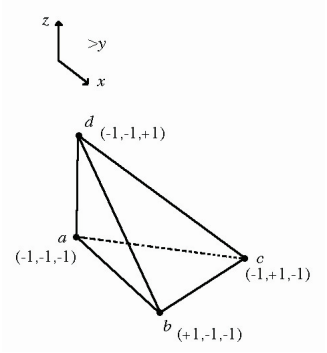


Figure 5.11: Reverse-slip: PyLith-GeoFEST comparison of displacement residuals on a 500m resolution mesh (left: t=5 years, right: t=10 years).

Appendix A

Shape Functions

A.1 Linear Tetrahedral Element (tet4)



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

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 5.2.

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

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

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

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

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

Rearranging terms, we get

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

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

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	$+\frac{1}{2}$

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

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

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

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

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

Appendix B

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