

HiQLab: User's Manual

David Bindel and Tsuyoshi Koyama

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1 Introducing HiQLab

1.1 HiQLab description

Electromechanical resonators and filters, such as quartz, ceramic, and surface-acoustic wave devices, are important signal-processing elements in communication systems. Over the past decade, there has been substantial progress in developing new types of miniaturized electromechanical resonators using microfabrication processes. For these micro-resonators to be viable they must have high and predictable quality factors (Q). Depending on scale and geometry, the energy losses that lower Q may come from material damping, thermoelastic damping, air damping, or radiation of elastic waves from an anchor. While commercial finite element codes can calculate the resonant frequencies, they typically offer only limited support for computing damping effects; and even if the software is capable of forming the systems of equations that describe physically realistic damping, there may not be algorithms to quickly solve those equations.

HiQLab is a finite element program written to study damping in resonant MEMS. Though the program is designed with resonant MEMS in mind, the architecture is general, and can handle other types of problems. Most architectural features in HiQLab can be found in standard finite element codes like FEAP; we also stole liberally from the code base for the SUGAR MEMS simulator.

We wrote HiQLab to be independent of any existing finite element code for the following reasons:

- We want to share our code, both with collaborators and with the community. This is a much easier if the code does not depend on some expensive external package.
- We want to experiment with low-level details, which is more easily done if we have full access to the source code.
- We are mostly interested in linear problems, but they are problems with unusual structure. It is possible to fit those structures into existing finite element codes, but if we have to write new elements, new solver algorithms, *and* new assembly code in order to simulate anchor losses using perfectly matched layers, we get little added benefit to go with the cost and baggage of working inside a commercial code.
- We are still discovering which algorithms work well, and would like to be able to prototype our algorithms inside MATLAB. We also want to be able to run multi-processor simulations outside of MATLAB, both to solve large problems and to run optimization loops. FEMLAB supports a MATLAB interface, but in our experience does not deal well with large simulations. FEAP also supports a MATLAB interface (which we wrote), and the data structures in HiQLab and FEAP are similar enough that we can share data between the two programs.

The main drawback of developing a new code is that we lack the pre- and post-processing facilities of some other programs.

1.2 HiQLab architecture

The main components of HiQLab are as follows.

- The mesh description language

The main way to describe devices in HiQLab is to write a mesh input deck using the Lua programming language (<http://www.lua.org>). Because meshes are generated programmatically, it is easy to create parameterized descriptions with hierarchies and arrays.

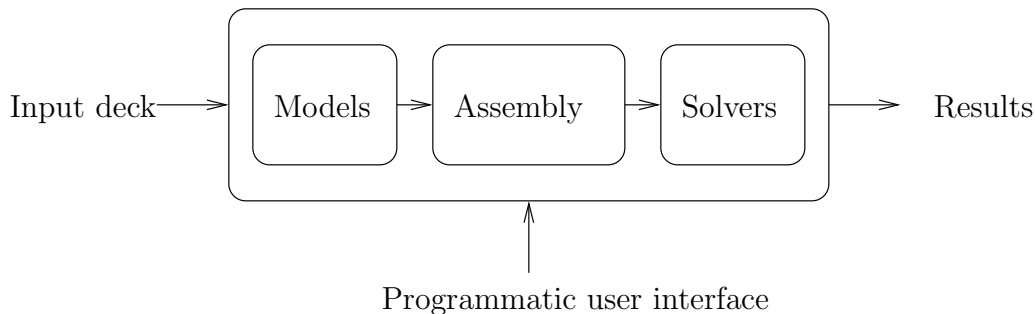


Figure 1: Architecture of HiQLab

- The programmatic user interfaces

There are two versions of the user interface: the MATLAB interface and the standalone interface. When using the MATLAB interface, a user has access to the full range of MATLAB's numerical solvers and graphics routines. When using the standalone interface, a user does not have as many built-in capabilities; but because the standalone interface does not rely on MATLAB, it takes less memory and can solve larger problems. Like the mesh description interface, the user interface is written in the Lua language, and is fully programmable. We describe both the MATLAB interface and the standalone interface in this manual.

- The element model library

The element library includes linear, quadratic, and cubic quad and brick elements for elastic problems and coupled thermoelastic problems in plane strain, plane stress, axisymmetry, or three dimensions. The code also provides scalar wave equation elements in one, two, or three dimensions. For both scalar and elastic waves, the code supports *perfectly matched layer* absorbing boundaries to mimic the effect of infinite domains.

- The solver library

The solver library includes code for

- Modal analysis of structures with anchor loss and thermoelastic damping.
- Forced response analysis, including forced response visualization and Bode plot construction. The forced response analysis routines incorporate reduced order models.

1.3 Download and basic setup

The fastest way to get started with HiQLab is to use the pre-compiled version, available for Linux or Windows machines. You can download the source code and pre-compiled executables at

<http://www.cs.berkeley.edu/~dbindel/hiqlab/>

If you wish to run HiQLab with the MATLAB interface, you will need MATLAB version 6 or later.

If you wish to build your own version of HiQLab, you will need

- A C/C++ compiler and a FORTRAN 77 compiler (we have used the GNU compiler on Linux and Windows, and the Intel compilers on Itanium)
- Perl 5.002 or later
- LAPACK and BLAS (Basic Linear Algebra Subroutine) libraries. If you are compiling the MATLAB front-end for HiQLab, these are already provided.
- UMFPACK (a linear system solver)
- ARPACK (an iterative eigenvalue solver)

If these packages are installed, you should be able to configure and compile the software by running the following commands from the HiQLab top-level directory:

```
./configure  
make
```

At the time this manual is being written, HiQLab is *alpha* software. The code is still changing rapidly, and if you have trouble setting up the program and running basic examples, please check to make sure you have the most recent version.

1.3.1 Running in MATLAB

Once you have downloaded the pre-compiled version of the code (or once you have built your own version), start MATLAB and run the file `init.m`. You should see something like the following:

```
< M A T L A B >  
Copyright 1984-2001 The MathWorks, Inc.  
Version 6.1.0.450 Release 12.1  
May 18 2001
```

To get started, type one of these: `helpwin`, `helpdesk`, or `demo`.
For product information, visit www.mathworks.com.

```
>> init  
HiQlab 0.2  
Copyright : Regents of the University of California  
Build system: i686-pc-linux-gnu  
Build date : Tue Mar 1 12:51:22 PST 2005  
Bug reports : dbindel@cs.berkeley.edu  
>>
```

You must run `init` before using HiQLab from MATLAB. The `init` script sets the MATLAB path variable so that MATLAB can find the files HiQLab needs for its analyses.

If you run `init` and see the HiQLab banner, that means that you have a working version of the MATLAB HiQLab interface for your machine. If there is an error message when you run `init`, please send an e-mail including the exact error message, operating system version, and MATLAB version.

1.3.2 Running in standalone mode

If you want to use the standalone version, look for an executable file called `hiqlab` in the `src/lua` subdirectory. When you run `hiqlab` with no arguments, you should see an banner with program information and a control prompt:

```
[dbindel@localhost lua]$ ./hiqlab
-----
HiQlab 0.2
Copyright   : Regents of the University of California
Build system: i686-pc-linux-gnu
Build date  : Thu Mar  3 19:29:03 PST 2005
Bug reports : dbindel@cs.berkeley.edu

Lua 5.0.2 Copyright (C) 1994-2004 Tecgraf, PUC-Rio
-----
```

>

To end the HiQLab session, press Ctrl-D on the keyboard. HiQLab may also be run non-interactively: if `batch.lua` is a script that runs an analysis and prints it out, for example, you might run

```
hiqlab batch.lua
```

Like the MATLAB interface, the standalone user interface needs to know where to find files. The `init.lua` file in the HiQLab main directory specifies these files. The first line of `init.lua` has the form

```
HOME='/my/hiq/directory'
```

where “my hiq directory” should be replaced by the directory where HiQLab is installed. This is usually done automatically at configuration time. You can ensure that HiQLab executes `init.lua` when it starts in one of two ways:

1. Set the `HIQ_INIT` environment variable to point to the full path for `init.lua`. HiQLab calls any files specified in the HiQLab directory
2. Specify `init.lua` using the `-l` argument to HiQLab. For example, to execute `init.lua` before running HiQLab in interactive mode,

```
hiqlab -l /my/hiq/directory/init.lua -i
```

and to run a batch script,

```
hiqlab -l /my/hiq/directory/init.lua batch.lua
```

1.4 “Hello world” in HiQLab

1.4.1 Describing a cantilever beam

Figure 2 shows the input file used to describe a simple cantilever beam. We now describe the input file in detail.

```
require 'common.lua'

l = 10e-6      -- Beam length
w = 2e-6      -- Beam width
dense = 0.5e-6 -- Approximate element size (for block generator)
order = 2     -- Order of elements

mesh = Mesh:new(2)
mat = make_material('silicon2', 'planestrain')
mesh:blocks2d( { 0, l }, { -w/2.0, w/2.0 }, mat )

mesh:set_bc(function(x,y)
  if x == 0 then return 'uu', 0, 0; end
end)
```

Figure 2: The complete mesh input file for a cantilever beam

- Including common support files:

```
require 'common.lua'
```

Typically, input files will start with one or more `require` statements, which are used to load function definitions, material databases, and other data. The `require` statement is much like an include statement in C or Fortran, except that `require` loads each file *once*. For example, the file `common.lua` begins by requiring `material.lua`; if my input file also started with a line `require 'material.lua'`, I would not end up with two copies of the material definitions file.

When the interpreter encounters a `require` statement, it searches through a standard path to find a file with a matching name. We will say more about the search path in Section 3.1. The file `common.lua`, which is defined in `models/common.lua` provides functions that are useful for defining element types; `common.lua` should be included in most mesh description files.

- Defining geometric parameters:

```
l = 10e-6      -- Beam length
w = 2e-6      -- Beam width
```

A two-dimensional beam model must have a length and a width. These two lines give the beam length (10 μm) and width (2 μm) in MKS units. Giving names to geometric parameters makes the input file easier to read than it would otherwise be. In Section ??, we describe how named parameters can be set from outside the input file in order to simplify parameter studies.

- Defining mesh generation parameters:

```
dense = 0.5e-6 -- Approximate element size (for block generator)
order = 2     -- Order of elements
```

The mesh file must describe both the geometry of the device and the parameters that define the mesh. HiQLab includes several functions that define regular “blocks” that can be tied together to form a mesh. The `dense` and `order` parameters control how HiQLab builds these blocks. The `order` parameter is the order of polynomial interpolation used within each element: linear, quadratic, and cubic elements are available. The `dense` parameter describes the element size.

- Creating a mesh object:

```
mesh = Mesh:new(2)
```

All information about the mesh is stored in a mesh object. The mesh constructor has a single argument, the dimension of the ambient space for the problem. The mesh object should be called `mesh`.

- Defining a material:

```
mat = make_material('silicon2', 'planestrain')
```

Build an element type for computing the response of silicon in plane strain. The first argument refers to an entry in `materials.lua` which defines material arguments like Young’s modulus and the Poisson ratio; subsequent arguments define the type of analysis (plane stress, plane strain, axisymmetric, or three-dimensional).

- Defining the mesh:

```
mesh:blocks2d( { 0, l }, { -w/2.0, w/2.0 }, mat )
```

The mesh for a cantilever beam is simple: it covers the rectangular region $[0, l] \times [-w/2, w/2]$. The `blocks2d` generator creates such a region and adds it to the mesh; the element size and order are determined by the global variables `dense` and `order` defined earlier, and the `mat` parameter from the previous line defines which material should be used.

- Defining boundary conditions:

```
mesh:set_bc(function(x,y)
  if x == 0 then return 'uu', 0, 0; end
end)
```

By calling `mesh:set_bc(myfunc)`, we define boundary conditions for the problem. `myfunc` may be an anonymous function (a function without an explicitly assigned name), which is what we use for this problem. The function is called at every node in the mesh. If the call returns nothing, then no boundary conditions are applied; otherwise, the call returns a string which defines whether essential or natural (displacement or flux) boundary conditions are applied. In this example, displacement boundary conditions (denoted by ‘u’) are given for both the x and y displacements. The two numeric arguments after the string indicate that the x and y displacements are set to zero.

1.4.2 Eigenvalue analysis in MATLAB

1.4.3 Eigenvalue analysis in standalone mode

1.5 Getting help

2 Basic features from Lua

Write about and or features!!

2.1 Variable types

Since Lua is a dynamically typed language, there are no type definitions in the language. In other words, the type is defined by the variable assigned. There are eight basic types in Lua. Of these the HiQLab user should be aware of the following 6.

1. **nil**: This is the type that is assigned to all variables by default. `nil` can be assigned to a variable as,

```
a = nil
```

2. **boolean**: This has two types, `true` and `false`. In Lua, any value may represent a condition. In conditionals, *ONLY* `false` and `nil` are considered false, and everything else is considered true. Beware that the value zero and empty string both represent *TRUE*.

3. **number**: Lua has only one number type, real double-precision floating point numbers. There are *NO* integer types. Valid types of number representations are,

```
4      0.4      4.57e-3    0.3e12    5e+20
```

4. **string**: Strings have the usual meaning, a sequence of characters. The string can be assigned by putting them between single quotes or double quotes. They can be assigned to a variable by the following statement.

```
a = "a line"
b = 'another line'
```

Strings in Lua can contain the following C-like escape sequences:

Table 1: C-like escape sequences

<code>\b</code>	: back space
<code>\n</code>	: newline
<code>\t</code>	: horizontal tab
<code>\v</code>	: vertical tab
<code>\\</code>	: back slash
<code>\'</code>	: single quote
<code>\"</code>	: double quote

Strings can be concatenated by the operator ...

```
a = "Hello"
b = "World"
c = a..b
d = a.." "..b
print(c)      --> HelloWorld
print(d)      --> Hello World
```

5. **table**: This type is used to implement associative arrays. An associative array is an array that can be indexed not only with numbers, but also with strings or any other value of the language. Moreover, tables have no fixed size, and the size is adjusted dynamically. Thus a single Lua table can contain different types of data.

```
a      = {}           -- create a table
a[1] = 4             -- store double
a[21]= 'Hello world' -- store string
print(a[1])         --> 4

a['A']  = a          -- Index with character
a['John'] = Doe      -- Index with string
print(a['John'])    --> Doe
print(a[John])     --> nil
```

Tables in Lua are treated as objects similar to Java. Thus a program that manipulates tables, only manipulates references or pointer to them.

```
b = a                -- the reference to the table that 'a'
                    -- points to is passed
```

Additionally, since tables are like objects, `a.name` can be used as syntactic sugar for `a["name"]`.

```
a      = {}
a["x"] = 4
print(a["x"])    --> 4
print(a.x)      --> 4
```

Tables can be initialised with values by the following argument, in which case the keys to the corresponding values start from one (and not with zero, as in C).

```
a      = { 10, 11, 12}
print(a[1])     --> 10
```

6. **function** This aspect will further be explained in section ????.

WHAT YOU SHOULD KNOW(Zentei Chishiki).

2.2 Ending a line

A statement in Lua is called a **chunk**, and is simply a sequence of statements. This **chunk** can take a single line, multiple lines, or can even span multiple files. A semicolon may optionally follow any statement, but this is just a convention. Thus, the following four chunks are equivalent.

```
-- Chunk 1
a = 1
b = a*2
```

```
-- Chunk 2
a = 1;
b = a*2

-- Chunk 3
a = 1; b = a*2

-- Chunk 4
a = 1 b = a*2
```

2.3 Print statement

All variable types can be printed to the screen through the command `print`

```
a = 4
print(a)    --> 4
b = "Hello World"
print(b)    --> Hello World
c = false
print(c)    --> false
d = {4, 5, 6}
print(d)    --> table: 0x8067d90
            (The reference is printed in this case)
print(d[2]) --> 5
```

2.4 Comments

A comment starts anywhere with a double hyphen (`-`) and runs until the end of the line. Lua also offers block comments, starting with `--[[` and run till `--]]`.

```
-- This is a commented line

--[[
    print(10)           --This is a commented block
--]]
```

2.5 For loops

for loops in Lua are stated by the following structure.

```
for var=start_value, end_value, increment do
    do something
end
```

The loop will execute `something` for each value of `var` from `start_value` to `end_value` with and increment of `increment`. If `increment` is absent, the increment will be assumed one.

An example for printing the numbers 1 through 10 is presented below.

```
for i=1,10 do
  print(i)
end
```

One remark that should be made is that in the example above the index i is declared as a local variable. This implies that once the for loop is terminated the value of i will not be retained and cannot be referenced to.

2.6 If statements

if statements in Lua are defined by the following structures.

```
if condition_expression then
  do something
end
```

or,

```
if condition_expression then
  do something
else
  do something else
end
```

All other values other than `false` or `nil` that are returned by the `condition_expression` will be treated as `true`.

An example code to print the larger of the value `a,b` is:

```
if a > b then
  print(a)
else
  print(b)
end
```

To avoid writing nested ifs, one can use `elseif` in the following structure.

```
if condition_expression then
  do something
elseif condition_expression
  do something else
else
  do yet something else
end
```

2.7 Functions

A function in Lua is defined by the following format.

```
function function_name(input_arguments)
  function_body
end
```

The input arguments can any type of Lua variable, and when multiple values are passed, they must be seperated by a comma. It is possible to assign no input arguments.

`function_body` will consist of the standard Lua chunks. For the function to return an output value the `return` command must be placed.

```
function function_name(input_arguments)
    function_body
    return output_arguments
end
```

`output_arguments` may return any type of Lua variable, and when multiple values are returned, they must be seperated by a comma.

An example of a function which takes two numbers `a,b` as the input and returns their sum is shown below.

```
function add(a,b)

    sum_ab = a + b

    return sum_ab
end
```

The method of calling this function is the following.

```
a = 4
b =-2.11
sum_ab = add(a,b)
print(sum_ab)      -> 1.89
```

The function above can be modified to also return the difference by the following code.

```
function add_diff(a,b)

    sum_ab = a + b
    diff_ab= a - b

    return sum_ab, diff_ab
end
```

The method of calling this function is the following.

```
a = 4
b =-2.11
sum_ab, diff_ab = add_diff(a,b)
print(sum_ab)      -> 1.89
print(diff_ab)     -> 6.11
```

3 Mesh description (Lua)

3.1 require statements and common files

Need directory tree diagram or something

Typically, mesh input files will start with one or more `require` statements, which are used to load function definitions, material databases, and other data. The `require` statement is much like an include statement in C or Fortran, except that `require` loads each file *once*. For example, the file `common.lua` begins by requiring `material.lua`; if my input file also started with a line `require 'material.lua'`, I would not end up with two copies of the material definitions file. When the interpreter encounters this `require` statement, it searches through a standard path to find a file with a matching name.

The file `common.lua`, which is defined in `models/common.lua` provides functions that are useful for defining element types; `common.lua` should be included in most mesh description files. The functions contained in `common.lua` are sorted by functionality and presented in table 2. Further details on the input and output arguments of the function are given in the section?? related with non-dimensionalization and section??? related with material models.

The file `material.lua`, which is defined in `models/material.lua` provides a material database which is useful for defining element types; `materials.lua` is automatically incorporated by including the file `common.lua`. The functions contained in `materials.lua` are sorted by functionality and presented in table 3. The materials in the database are sorted by the type of analysis they are capable of in table 4. Further details on the input and output arguments of the functions and properties of the materials are given in the section?? related with material models.

Table 2: Functions contained in `common.lua`

Functionality	Function name
Retrieve material property values	<code>get_material(mtype)</code>
Set characteristic scales for non-dimensionalization	<code>mech_nondim(mtype,cL)</code> , <code>ted_nondim(mtype,cL)</code> , <code>pz_nondim(mtype,cL)</code> , <code>em_nondim(mtype,cL,eps)</code>
Non-dimensionlize material properties	<code>mech_material_normalize(mtype)</code> , <code>ted_material_normalize(mtype)</code> , <code>pz_material_normalize(mtype)</code>
Construct element with <code>mtype</code> material property	<code>make_material(mtype,etype,wafer,angle)</code> , <code>make_material_te(mtype,etype,wafer,angle)</code> , <code>make_material_pz(mtype,etype,wafer,angle)</code> , <code>make_material_couple_em2d(eps,etype)</code>

Table 3: Functions contained in `materials.lua`

Functionality	Function name
Assign proper mechanical variables if non-existent	<code>fill_mech(mtype)</code>
Assign proper piezoelectric variables if non-existent	<code>fill_piezo(mtype)</code>

Table 4: Materials contained in `materials.lua`

Material name	Crystal	Analysis			
		mech	thermoelastic	piezo	electromech
<code>sc_silicon</code>	cubic	○	○	×	○
<code>poly_silicon</code>	isotropic	○	○	×	○
<code>amor_silicon</code>	cubic	○	○	×	○
<code>silicon</code>	isotropic	○	×	×	○
<code>silicon2</code>	isotropic	○	○	×	○
<code>hfo2</code>	isotropic	○	×	×	○
<code>sic</code>	isotropic	○	×	×	○
<code>sige</code>	isotropic	○	×	×	○
<code>siox</code>	isotropic	○	×	×	○
<code>diamond</code>	isotropic	○	×	×	○
<code>aln</code>	hexagonal	○	×	○	×
<code>aln_isotropic</code>	isotropic	○	×	○	×
<code>aln_piazza</code>	hexagonal	○	×	○	×
<code>pt_piazza</code>	isotropic	○	×	×	○
<code>al_piazza</code>	isotropic	○	×	×	○

3.2 Constructing the Mesh object

All the information about the mesh is stored in a mesh object. The mesh constructor has a single argument, the dimension of the ambient space for the problem.

`Mesh(ndm)` A mesh object with `ndm` dimensions for the ambient space.

The mesh object should be called `mesh`. The mesh is usually constructed by the following statement.

```
mesh = Mesh:new(ndm)
```

3.3 Adding nodes

Nodal points must be defined in order to construct the mesh. There are two primitive operations to add nodes to the mesh geometry.

`add_node(x)` Adds a single node with positions listed consecutively in the array `x={x1,y1}`, and returns the identifier of the node.

`add_node(x,n)` Adds `n` nodes with positions listed consecutively in the array `x={x1,...,xn}`, and returns the identifier of the first node.

It must be noted that the identifier of the nodes are 0 based in the Lua environment. Thus the the identifier returned after adding the very first node will be `0`.

The nodes can be added to `mesh` by the following statements.

```
x = {x1, y1,  
      x2, y2,  
      x3, y3}
```

```
identifier_for_first_node = mesh:add_node(x,3)
```

3.4 Adding elements

3.4.1 Element types

HiQLab currently supports line, quad, and brick elements for mechanical, thermomechanical, piezoelectric mechanical, and electromechanical problems. Details of implementation and capabilities of each element are noted in section 5, which explains the element library.

3.4.2 Line, quad, and brick node ordering

The current shape function library supports linear, quadratic, and cubic; and bilinear, biquadratic, and bicubic quads; and trilinear, triquadratic, and tricubic bricks. The ordering is non-standard. For lines, the nodes are listed in increasing order starting from one end node. This is shown in Figure 3.

For quads, the nodes are listed in increasing order by their coordinates, with the y coordinate varying fastest. For example, for 4-node,9-node, and 16-node quads, we use the ordering shown in Figure 4.

The ordering in the 3D brick case is similar, but with the z coordinate varying fastest, the y coordinate second-fastest, and the x coordinate most slowly. For example, for 8-node and 27-node bricks, we use the ordering shown in Figure 5.

So long as the ordering in the spatial domain is consistent with the ordering in the parent domain, the isoparametric mapping will be well-behaved (so long as element distortion is not too great). The `add_block` commands described in the section 3.5 produce node orderings which are consistent with our convention.

The primary advantage of the node ordering we have chosen is that it becomes trivial to write loops to construct 2D and 3D tensor product shape functions out of simple 1D Lagrangian shape functions. Also, it becomes simple to write the loops used to convert a mesh of higher order elements into four-node quads or eight-node bricks for visualization (see Section ??).

Development note: Currently, the number of Gauss points used by the element library is fixed at compile time. It might be wise to allow the user to change that.

3.4.3 Adding elements to mesh

In order to add an element to the mesh, we must first construct an element object. This can be done by the following statement.

```
etype = mesh:Element(arguments)
```

To construct a `PMLElastic2D` element, `Element` is replaced by the following,

```
etype = mesh:PMLElastic2d( E, nu, rho, analysis_type);
```

Once this element object is constructed we must define the connectivity of a particular element and add this to the `mesh` object by the command:

```
add_element(con,etype,nen,num) Adds n elements of type etype with node lists of length nen listed consecutively in the array con, and returns the identifier of the first element added.
```

It must be noted that the identifier of the elements are 0 based in the Lua environment. Thus the the identifier returned after adding the very first element will be 0.

A sample code for adding one 4-noded quad element to the mesh would look like,

```
con = { node_num1, node_num2, node_num3, node_num4}
identifier_for_first_element = mesh:add_element(con, etype, 4, 1)
```

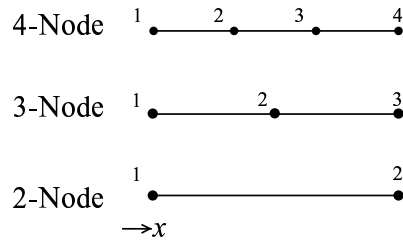


Figure 3: Node ordering for 2-node, 3-node, and 4-node line elements

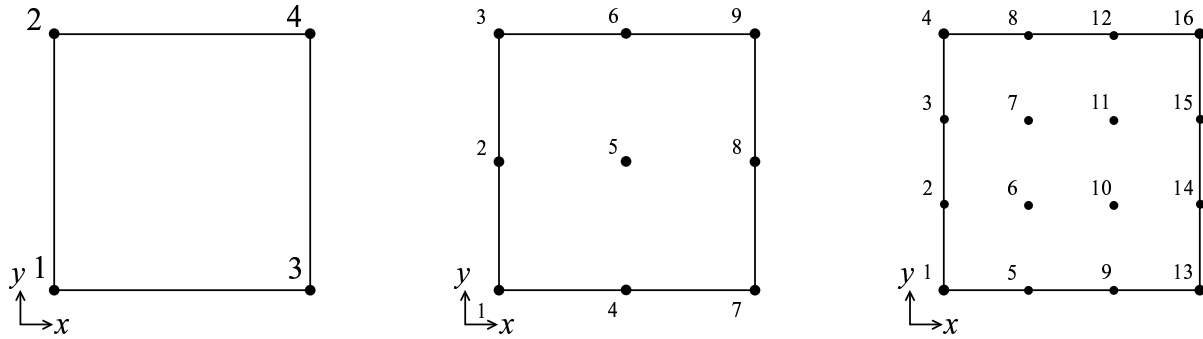


Figure 4: Node ordering for 4-node, 9-node, and 16-node quads

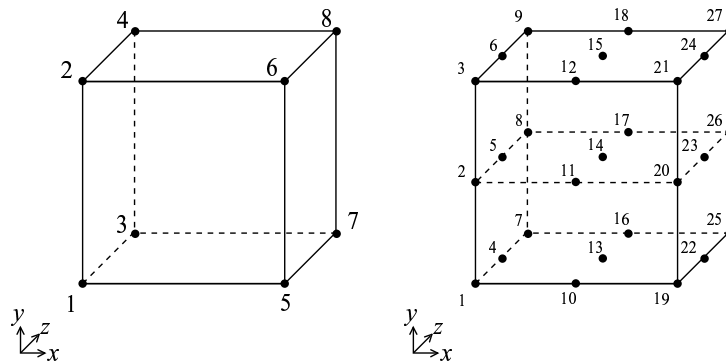


Figure 5: Node ordering for 8-node and 27-node brick

3.5 Block generators

Though the methods introduced above for adding nodes and elements are general, they can be tedious to use when defining complicated geometry or for parametric mesh refinement analyses. Mesh generation can be simplified by using the block generator commands introduced in this section.

3.5.1 Simple block generators

`add_block(x1,x2,nx,etype,order)` The `add_block` methods allow you to add a Cartesian strip of elements. This method takes two end points `x1,x2` and the number of points along the edge (including end points), and constructs a mesh of the strip $[x_{\min}, x_{\max}] \times$. It is possible to remap the bricks later by directly manipulating the mesh `x` array. Each element has a specified order, and the number of points along each edge should be one greater than a multiple of that order. Thus `nx` and `order` should satisfy the relation,

$$nx = \text{order} \times (\text{number of elements between end points}) + 1$$

The case where we have 7 nodes (`nx=7`) with varying order of elements is shown in Figure 6.

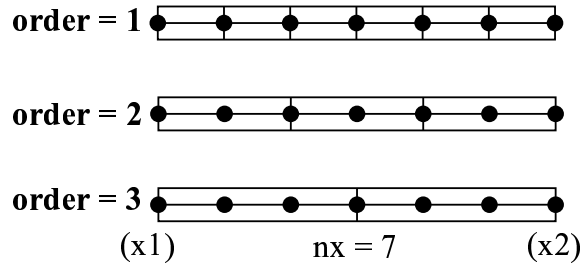


Figure 6: `add_block(x1,x2,nx=7,etype,order=1,2,3)`

`add_block(x1,y1,x2,y2,nx,ny,etype,order)` This is a 2D version of the `add_block` generator.

The case where we have 7 nodes (`nx=7`) by 3 nodes (`ny=3`) with varying order of elements is shown in Figure 7. We see here in this case that `nx,ny` both must satisfy the relation,

$$\begin{aligned} nx &= \text{order} \times (\text{number of elements between end points}) + 1 \\ ny &= \text{order} \times (\text{number of elements between end points}) + 1 \end{aligned}$$

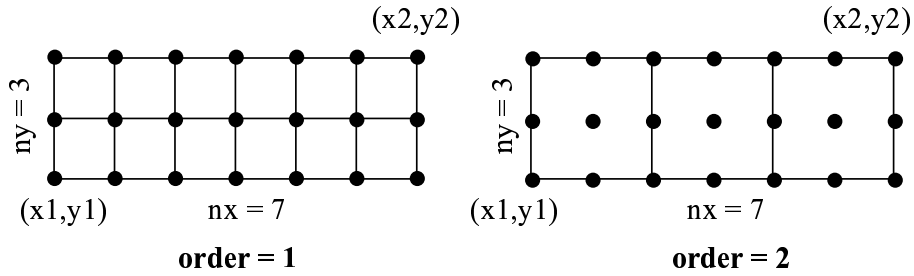


Figure 7: `add_block(x1,y1,x2,y2,nx=7,ny=3,etype,order=1,2)`

`add_block(x1,y1,z1,x2,y2,z2,nx,ny,nz,etype,order)` This is a 3D version of the `add_block` generator.

3.5.2 Multiple block generators

The block generators listed in this section can be understood as conducting multiple `add_blocks` simultaneously. This is done by passing an array of controls points along each edge, and specifying the number of nodes along the edge between these control points.

`blocks1dn(xlist,rlist,etype,order)` Creates a 1D strip of elements with specified nodes along the edge $xlist=\{x_1, \dots, x_m\}$, and specified number of nodes along the edge between specified nodes $rlist=\{r_1, \dots, r_{m-1}\}$. $r_k(k = 1, \dots, m - 1)$ and `order` must satisfy the relation stated in the generator `add_block`.

The case where we have 3 control nodes, with 5 and 3 nodes along the edges between these nodes and varying order of elements, is shown in Figure 8.

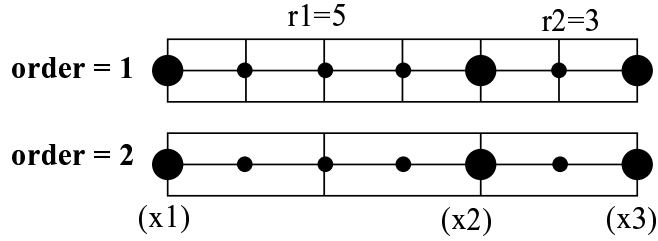


Figure 8: `blocks1dn(\{x1,x2,x3\},\{r1=5,r2=3\},etype,order=1,2)`

`blocks2dn(xlist,rlist,ylist,slist,etype,order)` Creates a 2D block of elements with specified nodes along the edges $xlist=\{x_1, \dots, x_m\}$, $ylist=\{y_1, \dots, y_n\}$, and specified number of nodes along each edge between specified nodes $rlist=\{r_1, \dots, r_{m-1}\}$, $slist=\{s_1, \dots, s_{n-1}\}$. Both $r_k(k = 1, \dots, m - 1)$, $s_k(k = 1, \dots, n - 1)$ and `order` must satisfy the relation stated in the generator `add_block`.

`blocks3dn(xlist,rlist,ylist,slist,zlist,tlist,etype,order)` Creates a 3D block of elements with specified nodes along the edges $xlist=\{x_1, \dots, x_m\}$, $ylist=\{y_1, \dots, y_n\}$, $zlist=\{z_1, \dots, z_p\}$, and specified number of nodes along each edge between specified nodes $rlist=\{r_1, \dots, r_{m-1}\}$, $slist=\{s_1, \dots, s_{n-1}\}$, $tlist=\{t_1, \dots, t_{p-1}\}$. Both $r_k(k = 1, \dots, m - 1)$, $s_k(k = 1, \dots, n - 1)$, $t_k(k = 1, \dots, p - 1)$ and `order` must satisfy the relation stated in the generator `add_block`.

`blocks1d(xlist,etype,order,dense1)` Creates a 1D strip of elements with specified nodes along the edge `xlist={x1,...,xm}`. Nodes are inserted between these nodes according to the parameter `dense1`, which specifies the approximate size of the element. The method will fit r_k number of elements with `order` between the specified nodes, where r_k ($k = 1, \dots, m - 1$) is defined by the equation,

$$r_k = \text{order} * \text{ceil} \left(\frac{x_{k+1} - x_k}{\text{dense1}} \right) + 1 .$$

The function `ceil` rounds to the nearest integer towards infinity. If the parameter `order` or `dense1` is not specified, the method will look for a global variable with the name `order` and `dense`. If these are supplied, the method will execute with no error.

The case where we have 3 control nodes with specified `dense1` is shown in Figure 9. Since the number of elements is specified by `dense1`, we can see that as we increase the order of each element, the number of nodes increases.

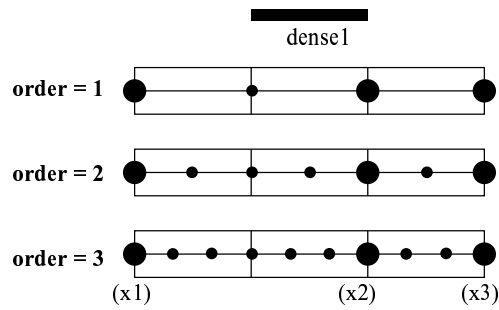


Figure 9: `blocks1d(x={x1,x2,x3},etype,order=1,2,3,dense1)`

`blocks2d(xlist,ylist,etype,order,dense1,dense2)` Creates a 2D block of elements with specified nodes along the edge `xlist={x1,...,xm}`, `ylist={y1,...,yn}`. Nodes are inserted between these nodes according to the parameter `dense1,dense2`, which specify the approximate size of the element. The method will fit r_k number of elements in the x direction with `order` between the specified nodes, and s_k number of elements in the y direction with `order` between the specified nodes, where r_k ($k = 1, \dots, m - 1$), s_k ($k = 1, \dots, n - 1$) is defined by the equation,

$$r_k = \text{order} * \text{ceil} \left(\frac{x_{k+1} - x_k}{\text{dense1}} \right) + 1$$

$$s_k = \text{order} * \text{ceil} \left(\frac{y_{k+1} - y_k}{\text{dense2}} \right) + 1 .$$

The function `ceil` rounds to the nearest integer towards infinity. If the parameter `order` or `dense1` `dense2` is not specified, the method will look for a global variable with the name `order` and `dense`. If these are supplied, the method will assume `order = order`, `dense1 = dense`, and `dense2 = dense` and execute with no error.

The case where we have 3 control nodes along the x direction and 2 control nodes along the y direction with specified `dense1,dense2` is shown in Figure 11. Since the number of elements is specified by `dense1,dense2`, we can see that as we increase the order of each element, the number of nodes increases.

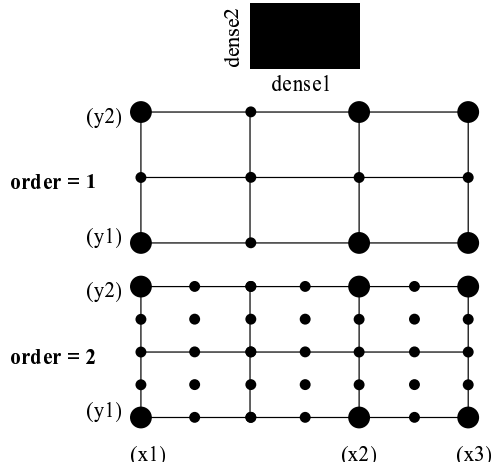


Figure 10: `blocks2d(m=3,n=4,etype,order=1,func)`

Figure 11: `blocks2d(x={x1,x2,x3},y={y1,y2},etype,order=1,2,dense1,dense2)`

`blocks3d(xlist,ylist,zlist,etype,order,dense1,dense2,dense3)` Creates a 3D block of elements with specified nodes along the edge. 3D version of the function above.

3.5.3 Transformed block generation in Lua

The block generators introduced in the previous two sections are limited to constructing square rectangular mesh regions which lacks flexibility. The generators presented in this section are versions of the `add_block` command which can construct curved or non-rectangular blocks.

`add_block_shape(m,n,p,etype,order,pts)` Creates a 3D (or 2D if `p` is omitted) quad block with node positions on $[-1, 1]^n dm$ and transforms them using an isoparametric mapping with points specified in the `pts` array. For example, for `pts = {0,0, 0,1, 1,0, 1,1}`, we would get a mesh for $[0, 1]^2$. `m,n,p` and `order` must satisfy the relation stated in the generator `add_block`.

An example of a $[-1, 1]^2$ region with 3 nodes along the x direction and 4 nodes along the y direction mapped to a 4-noded polygon with specified nodal points is presented in Figure 12.

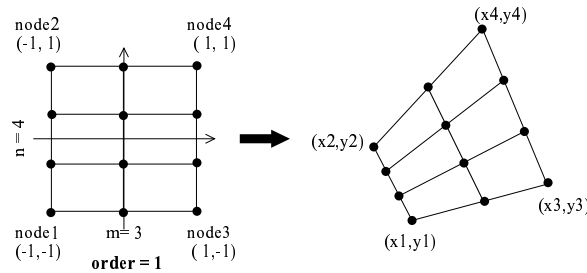


Figure 12: `add_block_shape(m=3,n=4,etype,order=1,pts)`

`add_block_transform(m,n,p,etype,order,func)` Creates a 3D (or 2D if `p` is omitted) quad block with node positions on $[-1, 1]^n dm$ and transforms them using the specified function. The function `func` must have the following form for 2D,

```
function func(x,y)
  -- Compute mapped coordinates (new_x,new_y) from (x,y)
  return new_x,new_y
end
```

and for 3D,

```
function func(x,y,z)
  -- Compute mapped coordinates (new_x,new_y,new_z) from (x,y,z)
  return new_x,new_y,new_z
end
```

`m,n,p` and `order` must satisfy the relation stated in the generator `add_block`.

An example of a $[-1, 1]^2$ region with 3 nodes along the x direction and 4 nodes along the y direction mapped to a curved block according to a polar mapping is presented in Figure 13.

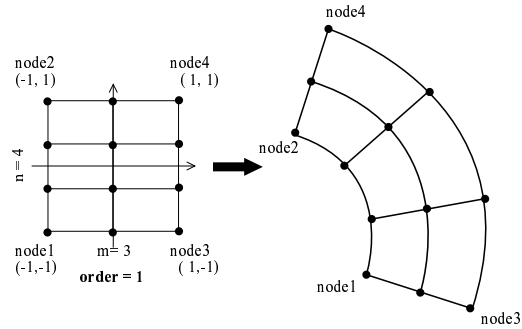


Figure 13: `add_block_transform(m=3,n=4,etype,order=1,func)`

`add_curved_block_shape2d(m,n,etype,order,pts,curv)` Creates a 2D quad block with nodes positions on $[-1, 1]^2$, m node points along the x direction and n node points along the y direction, both including edge points. m, n and $order$ must satisfy the relation stated in the generator `add_block`. The nodes on the corner of the quad block are mapped to the 4 node points stored in the table `pts={x1,y1,x2,y2,x3,y3,x4,y4}`. The table `curv={curv1,curv2,curv3,curv4}` contains the curvature on each edge, positive values specifying outward curvature and negative values inward curvature. m, n and $order$ must satisfy the relation stated in the generator `add_block`.

An example of a $[-1, 1]^2$ region with 3 nodes along the x direction and 4 nodes along the y direction mapped to a curved block with 4 control nodes and various curvatures on the edges is presented in Figure 14.

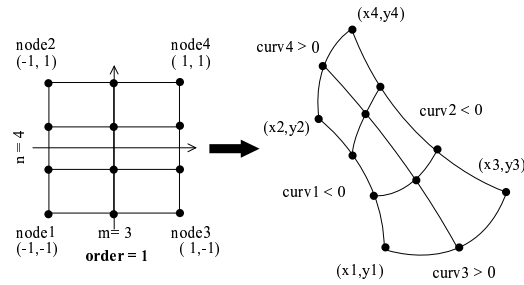


Figure 14: `add_curved_block_shape2d(m=3,n=4,etype,order=1,pts,curv)`

3.6 Tie command

The mesh class also has a `tie` method which “merges” nodes which are close to each other.

`tie(tol)` The `tie` method takes a tolerance `tol` to try to tie nodes together. If this argument isn’t specified, the method will look for a global parameter named `meshtol`. When this is given, the method will execute without error. If `tie` finds that nodes i and j in the specified range are within the given tolerance of each other, the `ix` array is rewritten so that references to either i or j become references to $\min(i, j)$.

The `tie` method acts as though the relation “node i is within the tolerance of node j ” were an equivalence relation. But while this relation is reflexive and symmetric, it does *not* have to be transitive for general meshes: that is, if x_i , x_j , and x_k are three node positions, you might have

$$\|x_i - x_j\| < \text{tol} \text{ and } \|x_j - x_k\| < \text{tol} \text{ and } \|x_i - x_k\| > \text{tol}.$$

The behavior of the `tie` algorithm is undefined in this case. Make sure it does not happen in your mesh.

Development note: The right thing to do here is to make the semantics explicit (by using the transitive closure of the above relationship, for instance) and warn the user if there were any places where the behavior of the `tie` command is not obvious.

3.7 Applying boundary conditions

There are three types of boundary conditions that can be set.

- Nodal boundary conditions: These are set on the degrees of freedom of each node in the mesh.
- Global variable boundary conditions: These are set on the global degrees of freedom that can be set. (See section on global variables for details).
- Element variable boundary conditions: These are set on the variables that pertain to a specific element.

For each case they are set by specifying functions and passing them into the mesh through the command,

`set_bc(func)` Passes a single nodal boundary condition function `func`.

`set_bc(func_table)` Passes a table of nodal boundary condition functions `func_table={func1, ..., funcn}`.

`set_globals_bc(func)` Passes a single global variable boundary condition function `func`.

`set_globals_bc(func_table)` Passes a table of global variable boundary condition functions `func_table={func1, ..., funcn}`.

`set_elements_bc(func)` Passes a single element variable boundary condition function `func`.

`set_elements_bc(func_table)` Passes a table of element variable boundary condition functions `func_table={func1, ..., funcn}`.

3.7.1 Nodal boundary conditions

The Lua function passed to `set_bc` should take as input the coordinates of the nodal point (the number depends on `ndm`), and should return a string describing which variables at that node are subject to force or displacement boundary conditions. If there are any nonzero boundary conditions, they should be specified by additional return arguments. For example, the following function applies zero displacement boundary conditions to the first degree of freedom and nonzero force conditions (of -1) to the third degree of freedom along the line $x = 0$:

```
function bcfunc(x,y)
  if x == 0 then return 'u f', 0, -1; end
end
```

If no boundary condition is specified (as occurs at $x \neq 0$ in the above example), then we assume that there is no boundary condition. If a boundary condition *is* specified, but without a specific value, then we assume the corresponding force or displacement should be zero. Run time errors result in a user warning, as described in Section ??.

The `bcfunc` defined above is passed to the mesh through the sample code,

```
mesh:set_bc(bcfunc)
```

3.7.2 Global variable boundary conditions

The Lua function passed to `set_globals_bc` should take as input the index of the global variable. This index is returned when the global variable is set to the mesh with the function `add_global`. (See section on global variables for details.) The function should return a string describing whether the global variable is subject to a force or displacement boundary condition. If there are any nonzero boundary conditions, they should be specified by additional return arguments. For example, the following function applies zero displacement boundary conditions to the global variable with index equal to 3:

```
function global_variable_bcfunc(ind)
  if ind == 3 then return 'u', 0; end
end
```

If no boundary condition is specified then we assume that there is no boundary condition. If a boundary condition *is* specified, but without a specific value, then we assume the corresponding force or displacement should be zero. Run time errors result in a user warning, as described in Section ??.

The `global_variable_bcfunc` defined above is passed to the mesh through the sample code,

```
mesh:set_globals_bc(global_variable_bcfunc)
```

3.7.3 Element variable boundary conditions

The Lua function passed to `set_elements_bc` should take as input the number of the element. This number is returned when the element is set to the mesh with the function `add_element`. (See section on elements for details.) The function should return a string describing whether the element variables are subject to a force or displacement boundary condition. If there are any nonzero boundary conditions, they should be specified by additional return arguments. For example, the following function applies a unit forced boundary conditions to the 2nd element variable of element number 42:

```
function element_variable_bcfunc(elemnum)
  if elemnum == 42 then return ' f', 1; end
end
```

If no boundary condition is specified then we assume that there is no boundary condition. If a boundary condition *is* specified, but without a specific value, then we assume the corresponding force or displacement should be zero. Run time errors result in a user warning, as described in Section ??.

The `element_variable_bcfunc` defined above is passed to the mesh through the sample code,

```
mesh:set_elements_bc(element_variable_bcfunc)
```

3.8 Helper Lua commands

3.8.1 Numerical value comparison commands

The methods stated here exist to mitigate the error introduced by numerical roundoff errors. When defining parameters and nodes for mesh information, addition, multiplication, and division give rise to situations where a variable x and y take the value,

```
x = 4.0
y = 4.0000000000000003
```

If we compare these two values, the statement

```
x == y
```

will return false, though actually they are the same value to the extent that we are interested in. Comparisons of numerical values such as these arise in boundary condition functions, pml stretch functions, and many more and can cause error. This can be alleviated by using the following comparison functions which take a certain tolerance in the comparison. For each function, if `tol` is not specified, it will search for a global variable named `meshtol`. If this variable is found the function will execute properly.

`mesheq(x,y,tol)` Returns true if $|x - y| < \text{tol}$ and false otherwise.

`meshleq(x,y,tol)` Returns true if $x < y + \text{tol}$ and false otherwise.

`meshsl(x,y,tol)` Returns true if $x < y - \text{tol}$ and false otherwise.

`meshgeq(x,y,tol)` Returns true if $x + \text{tol} > y$ and false otherwise.

`meshsg(x,y,tol)` Returns true if $x - \text{tol} > y$ and false otherwise.

`meshbetween(x,xmin,xmax,tol)` Returns true if $xmin - \text{tol} < x < xmax + \text{tol}$ and false otherwise.

`meshsbetween(x,xmin,xmax,tol)` Returns true if $xmin + \text{tol} < x < xmax - \text{tol}$ and false otherwise.

4 Global variables

4.1 Concept of a global variable

Introducing a global variable can be understood as a means to specify constraints among individual nodal degrees of freedom much like a lagrange multiplier. It allows one to specify a mode shape for selected nodal degrees of freedom and assigns a general degree of freedom for that mode.

The following simple example of a three degree of freedom spring mass mechanical system may clarify this concept. The equation of motion for the system can be written as,

$$\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix} \begin{pmatrix} \ddot{u}_1(t) \\ \ddot{u}_2(t) \\ \ddot{u}_3(t) \end{pmatrix} + \begin{bmatrix} k_1 + k_2 & -k_2 & 0 \\ -k_2 & k_2 + k_3 & -k_3 \\ -k_2 & k_2 - k_3 & k_3 \end{bmatrix} \begin{pmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \end{pmatrix} = \begin{pmatrix} F_1(t) \\ F_2(t) \\ F_3(t) \end{pmatrix} \quad (1)$$

or in more compact form,

$$\mathbf{M}\ddot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) = \mathbf{F}(t) \quad (2)$$

If we assume that the 2 and 3 degrees of freedom are connected by a rigid element, then the degrees of freedom can be expressed by one general degree of freedom as follows,

$$\begin{aligned} \begin{pmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \end{pmatrix} &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} u_1(t) + \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} z(t) \\ &= \mathbf{e}_1 u_1(t) + \mathbf{V}_z z(t) \\ &= [\mathbf{e}_1 \quad \mathbf{V}_z] \begin{pmatrix} u_1(t) \\ z(t) \end{pmatrix} \\ &= \mathbf{W} \begin{pmatrix} u_1(t) \\ z(t) \end{pmatrix} \end{aligned} \quad (3)$$

Inserting this expression and restricting the error to be orthogonal to this subspace spanned by the column vectors of \mathbf{W} results in the two degree of freedom system,

$$\mathbf{W}^* \mathbf{M} \mathbf{W} \begin{pmatrix} \ddot{u}_1(t) \\ \ddot{z}(t) \end{pmatrix} + \mathbf{W}^* \mathbf{K} \mathbf{W} \begin{pmatrix} u_1(t) \\ z(t) \end{pmatrix} = \mathbf{W}^* \mathbf{F}(t) \quad (4)$$

that must be solved.

4.2 Creating and defining global variables

The key to creating a global variable is to construct the shape vector \mathbf{V}_z pertaining to the global variable. This is conducted by specifying a function which is evaluated at each nodal degree of freedom, similar to the form of the nodal boundary conditions without the initial string. There is also an additional restriction that a number must be assigned for each nodal degree of freedom. As an example the shape function for the first example would have the form,

```
function shape_func_global_variable(x)
    if x==2 then return 1; end
    if x==3 then return 1; end
end
```

The general constructor for adding global variables to the mesh is:

`index = Mesh:add_global(shapeg,s_1,s_2)` `shapeg` must be a function of the form presented above. The variables `s_1,s_2` are optional and are the nondimensionalization parameters for the global variable. They can be numbers or strings that are predefined in the table `dim_scales`. (See section on non-dimensionalization for details). The function returns the `index` of the global variable.

`Mesh:set_globals()` Once all the global variables required are added they must be set to the mesh. Unless this function is called, the process will not be complete.

For the case presented in the previous section adding the global variable would take the process,

```
index = mesh:add_global(shape_func_global_variable,'L','F')
mesh:set_globals()
```

The value for the strings 'L' and 'F' must be set in `dim_scales`.

5 Element library

5.1 PML elements

Perfectly matched layers (PMLs) are what is used to model the effect of energy loss through supports or anchor loss. PMLs mimic the effect of an infinite or semi-infinite medium, by applying complex-value coordinate transformations. PMLs fit naturally into a finite element framework, but to implement them, we need some way to describe the exact form of the coordinate transformation. This coordinate-stretching function used in a PML is defined as a Lua function and set to the element that the PML is imposed by the following function:

`set_stretch(stretch_func)` Use a Lua function `stretch_func` to describe the coordinate transformation. The coordinate stretching function in 2D should have the form

```
function stretch_func(x,y)
  -- Compute stretching parameters sx and sy
  return sx, sy
end
```

If no stretch values are returned, they are assumed to be zero. The PML element should stretch the x and y coordinates by $(1 - is_x)$ and $(1 - is_y)$, respectively. The 3D case is handled similarly.

This function is set to the element in the following manner.

```
element_to_apply_pml:set_stretch(stretch_func)
```

The stretching function is only ever evaluated at node positions.

If there are no calls to either form of `set_stretch`, the PML element does not stretch the spatial coordinate at all, and so the element behaves exactly like an ordinary (non-PML) element.

For the exact form of this coordinate transformation function and details in implementation, see the PML example in the Examples Manual.

5.2 Laplace elements

The `PMLScalar1d`, `PMLScalar2d`, `PMLScalar3d`, and `PMLScalarAxis` classes implement scalar wave equation elements with an optional PML. The general constructor takes the form,

```
etype = make_material_s(mtype,analysistype)
```

The variable `mtype` must contain the fields `rho`(mass density) and `E`(material stiffness). The variable `analysis_type` can take one of the following strings,

- `1d`: 1 dimensional analysis
- `2d`: 2 dimensional analysis
- `3d`: 3 dimensional analysis
- `axis`: Axis symmetric analysis

The scalar wave equation has the form,

$$\rho \frac{\partial^2 u}{\partial t^2} = \nabla \cdot (\boldsymbol{\kappa} \nabla u) \quad (5)$$

where u is the scalar displacement, ρ is the density, and $\boldsymbol{\kappa}$ is the stiffness. If no coordinate stretching is defined, the elements will generate standard (real) mass and stiffness matrices. The class provides the following constructors:

`PMLScalar1d(kappa,rho)` Creates an isotropic 1D scalar wave equation element with material property κ and mass density ρ .

`PMLScalar2d(kappa,rho)` Creates an isotropic 2D scalar wave equation element with material property κ and mass density ρ .

`PMLScalar2d(D,rho)` Creates a 2D anisotropic element with a 2-by-2 property matrix D . Other than the material properties, this constructor is identical to the previous one.

`PMLScalarAxis(kappa,rho)` Creates an isotropic axisymmetric scalar wave equation element with material property κ and mass density ρ .

`PMLElasticAxis(D,rho)` Creates a 2D anisotropic element with a 2-by-2 property matrix D . Other than the material properties, this constructor is identical to the previous one.

`PMLScalar3d(kappa,rho)` Creates an isotropic 3D scalar wave equation element with material property κ and mass density ρ .

`PMLScalar3d(D,rho)` Creates a 3D anisotropic element with a 3-by-3 property matrix D . Other than the material properties, this constructor is identical to the previous one.

5.3 Elastic elements

The `PMLElastic2d`, `PMLElastic3d`, and `PMLElasticAxis` classes implement elasticity (Solid) elements with an optional PML transformation. The general constructor takes the form,

```
etype = make_material_e(mtype,analysistype)
```

`etype = make_material_e(mtype, etype, wafer, angle)` Constructs and returns a `PMLElastic` element, depending on the given arguments. The material type `mtype` (string or table containing material mechanical properties) and element type `etype(planestrain,planestress,axis,3d)` must be given. The arguments defining wafer orientation `wafer('100' or '111')` and orientation angle `angle [rad]` are optional. The table of mechanical properties `mtype` should contain the fields `rho`, `E`, `nu` for isotropic material, and `lambda`, `mu`, `alpha` for cubic material. (Currently this element can only treat cubic and isotropic mechanical material).

The variable `mtype` must be an elastic material containing different fields depending on the symmetry of the crystal considered. In the case of anisotropic material the second constructor is used, which defines the wafer orientation and angle. The variable `analysis_type` can take one of the following strings,

- `planestrain`: 2 dimensional planestrain analysis
- `planestress`: 2 dimensional planestress analysis
- `3d`: 3 dimensional analysis
- `axis`: Axis symmetric analysis

These elements solve the following equation,

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma} \quad (6)$$

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon} \quad (7)$$

$$\boldsymbol{\varepsilon} = \nabla_{\text{sym}} \mathbf{u} \quad (8)$$

Here, ρ is the density, $\boldsymbol{\sigma}$ is the stress, \mathbb{C} is the material stiffness tensor, $\boldsymbol{\varepsilon}$ is the infinitesimal strain, and \mathbf{u} is the displacement vector. In the case of an isotropic material, \mathbb{C} will depend only on two variables: the Young's modulus E and Poisson ratio ν . Otherwise the material property can be expressed by a matrix via Voigt notation. (See section on material models for further information). If no coordinate stretching is defined, the elements will generate standard (real) mass and stiffness matrices. The classes provides the following constructors:

`PMLElastic2d(E,nu,rho,plane_type)` Creates a plane strain (`plane_type = 0`) or plane stress (`plane_type = 1`) isotropic elasticity element with Young's modulus `E`, Poisson ratio `nu`, and mass density `rho`.

`PMLElastic2d(D,rho)` Creates a 2D element with a 3-by-3 elastic property matrix `D`. Other than the elastic properties, this constructor is identical to the previous one.

`PMLElastic2d(lua_State* L, lua_Object func)` Creates a 2D element with material parameters defined by a Lua function `func`. This function is accessed via the Lua state `L`. `func` must take one of the following forms.

```
function material_function(x,y)
  -- Compute 3-by-3 elastic property matrix D and
  --           mass density rho
  return D, rho
end
```

or,

```
function material_function(x,y)
  -- Compute Young's modulus E, Poisson ration nu,
  --           mass density rho, and analysis plane_type
  return E, nu, rho, plane_type
end
```

`PMLElasticAxis(E,nu,rho)` Creates an isotropic axisymmetric elasticity element with Young's modulus `E`, Poisson ratio `nu`, and mass density `rho`.

`PMLElasticAxis(D,rho)` Creates an element with a 4-by-4 elastic property matrix `D`. Other than the elastic properties, this constructor is identical to the previous one.

`PMLElasticTAxis(E,nu,rho,ltheta)` Creates an isotropic axisymmetric elasticity element with Young's modulus `E`, Poisson ratio `nu`, mass density `rho`, and wave number `ltheta`.

`PMLElasticTAxis(D,rho,ltheta)` Creates an element with a 6-by-6(???) elastic property matrix `D`. Other than the elastic properties, this constructor is identical to the previous one.

`PMLElastic3d(E,nu,rho)` Creates an isotropic 3D elasticity element with Young's modulus `E`, Poisson ratio `nu`, and mass density `rho`.

`PMLElastic3d(D,rho)` Creates an element with a 6-by-6 elastic property matrix `D`. Other than the elastic properties, this constructor is identical to the previous one.

5.4 Thermoelastic Elements

The `PMLElastic2d_te`, `PMLElastic3d_te`, and `PMLElasticAxis_te` classes implement thermoelasticity (Solid) elements with an optional PML transformation. The general constructor takes the form,

```
etype = make_material_te(mtype,analysistype)
```

```
etype = make_material_te(mtype,analysistype,wafer,angle)
```

Constructs and returns a `PMLElastic_te` element, depending on the given arguments. The material type `mtype` (string or table containing material thermomechanical properties) and element type `etype(planestrain,planestress,axis,3d)` must be given. The arguments defining wafer orientation `wafer('100' or '111')` and orientation angle `angle` [rad] are optional. The table of thermomechanical properties `mtype` should contain the fields `rho`, `E`, `nu` for isotropic material, and `lambda`, `mu`, `alpha` for cubic material. For both cases it should contain the fields `at`, `cp`, `kt` and `T0`. (Currently this element can only treat cubic and isotropic thermomechanical material).

The variable `mtype` must be an elastic material containing different fields depending on the symmetry of the crystal considered. In the case of anisotropic material the second constructor is used, which defines the wafer orientation and angle. The variable `analysis_type` can take one of the following strings,

- `planestrain`: 2 dimensional planestrain analysis
- `planestress`: 2 dimensional planestress analysis
- `3d`: 3 dimensional analysis
- `axis`: Axis symmetric analysis

These elements solve the following coupled equation,

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma} \quad (9)$$

$$\rho c_v \dot{\theta} = \nabla \cdot (\boldsymbol{\kappa}_T \nabla \theta) - T_0 \dot{\boldsymbol{\varepsilon}} : \mathbb{C} : \boldsymbol{\alpha}_T \quad (10)$$

$$\boldsymbol{\sigma} = \mathbb{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha}_T \theta) \quad (11)$$

$$\boldsymbol{\varepsilon} = \nabla_{\text{sym}} \mathbf{u} \quad (12)$$

Here, ρ is the density, $\boldsymbol{\sigma}$ is the stress, \mathbb{C} is the material stiffness tensor, $\boldsymbol{\varepsilon}$ is the infinitesimal strain, \mathbf{u} is the displacement vector and θ is the temperature fluctuation from T_0 , which is the referential temperature. In the case of an isotropic material, \mathbb{C} will depend only on two variables: the Young's modulus E and Poisson ratio ν . In the case of a cubic material, it will depend on three variables: λ , μ , and α . In both cases the material property can be expressed by a matrix via Voigt notation. (See section on material models for further information). The constants related with the thermal field are, $\boldsymbol{\kappa}_T$ the thermal conductivity tensor, c_v the specific heat at constant volume, and $\boldsymbol{\alpha}_T$ which is the linear coefficient of thermal expansion tensor. If no coordinate stretching is defined, the elements will generate standard (real) mass and stiffness matrices. The classes provides the following constructors:

```
PMLElastic2d_te(E,nu,rho,at,cp,kt,T0,plane_type)
```

Creates a plane strain (`plane_type = 0`) or plane stress (`plane_type = 1`) isotropic thermoelasticity element with Young's modulus `E`, Poisson ratio `nu`, mass density `rho`, coefficient of thermal expansion `at`, thermal capacity at constant pressure `cp`, thermal conductivity at `kt`, and reference temperature `T0`.

- `PMLElastic2d_te(Db,rho,at,cp,kt,T0)` Creates a 2D element with a 4-by-4 thermoelastic property matrix D . Other than the thermoelastic properties, this constructor is identical to the previous one.
- `PMLElastic3d_te(E,nu,rho,at,cp,kt,T0)` Creates an isotropic 3D thermoelasticity element with Young's modulus E , Poisson ratio ν , mass density ρ , coefficient of thermal expansion α , thermal capacity at constant pressure c_p , thermal conductivity k , and reference temperature T_0 .
- `PMLElastic3d_te(Db,rho,at,cp,kt,T0)` Creates a 3D element with a 7-by-7 thermoelastic property matrix D . Other than the thermoelastic properties, this constructor is identical to the previous one.
- `PMLElasticAxis_te(E,nu,rho,at,cp,kt,T0)` Creates an isotropic axisymmetric elasticity element with Young's modulus E , Poisson ratio ν , mass density ρ , coefficient of thermal expansion α , thermal capacity at constant pressure c_p , thermal conductivity k , and reference temperature T_0 .
- `PMLElasticAxis_te(Db,rho,at,cp,kt,T0)` Creates an element with a 5-by-5 thermoelastic property matrix D . Other than the thermoelastic properties, this constructor is identical to the previous one.

5.5 Piezoelectric elements

The `PMLElastic2d_pz`, `PMLElastic3d_pz`, and `PMLElasticAxis_pz` classes implement piezoelectric elasticity (Solid) elements with an optional PML transformation. The general constructor takes the form,

```
etype = make_material_pz(mtype,analysistype)
```

`etype = make_material_pz(mtype,analysistype,wafer,angle)` Constructs and returns a `PMLElastic_pz` element, depending on the given arguments. The material type `mtype` (string or table containing material thermomechanical properties) and element type `etype`(`planestrain`,`planestress`,`2hd`,`3d`) must be given. The arguments defining wafer orientation `wafer`('100' or '111') and orientation angle `angle` [rad] are optional. The table of thermomechanical properties `mtype` should contain the fields `c11`, `c12`, `c13`, `c33`, `c55`, `d16`, `d31`, `d33`, `kds1`, `kds3` for a hexagonal material. (Currently this element can only treat hexagonal piezoelectric mechanical material).

The variable `mtype` must be an elastic material containing different fields depending on the symmetry of the crystal considered. In the case of anisotropic material the second constructor is used, which defines the wafer orientation and angle. The variable `analysis_type` can take one of the following strings,

- `planestrain`: 2 dimensional planestrain analysis
- `planestress`: 2 dimensional planestress analysis
- `3d`: 3 dimensional analysis
- `axis`: Axis symmetric analysis

These elements solve the following coupled equation,

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma} \quad (13)$$

$$0 = \nabla \cdot \mathbf{D} \quad (14)$$

$$\boldsymbol{\sigma} = \mathbb{C} : (\boldsymbol{\varepsilon} - \mathbf{d}^T \mathbf{E}) \quad (15)$$

$$= \mathbb{C} : \boldsymbol{\varepsilon} - \mathbf{e}^T \mathbf{E} \quad (16)$$

$$\mathbf{D} = \mathbf{d} : \boldsymbol{\sigma} + \boldsymbol{\kappa}_{d\sigma} \mathbf{E} \quad (17)$$

$$= \mathbf{e} : \boldsymbol{\varepsilon} + \boldsymbol{\kappa}_{d\varepsilon} \mathbf{E} \quad (18)$$

$$\boldsymbol{\varepsilon} = \nabla_{\text{sym}} \mathbf{u} \quad (19)$$

$$\mathbf{E} = -\nabla \phi \quad (20)$$

Here, ρ is the density, $\boldsymbol{\sigma}$ is the stress, \mathbb{C} is the material stiffness tensor, $\boldsymbol{\varepsilon}$ is the infinitesimal strain, \mathbf{u} is the displacement vector and ϕ is the voltage potential. In the case of an isotropic material, \mathbb{C} will depend only on two variables: the Youngs modulus E and Poisson ratio ν . In the case of a hexagonal material, it will depend on five variables: c_{11} , c_{12} , c_{13} , c_{33} , c_{55} . In both cases the material property can be expressed by a matrix via Voigt notation. (See section on material models for further information). The constants related with the electric field are, $\boldsymbol{\kappa}_{d\sigma}$ the permittivity tensor at constant stress, $\boldsymbol{\kappa}_{d\varepsilon}$ the permittivity tensor at constant strain, \mathbf{d} the piezoelectric strain coefficients, and \mathbf{e} the piezoelectric stress coefficients. If no coordinate stretching is defined, the elements will generate standard (real) mass and stiffness matrices. The classes provides the following constructors:

`PMLElastic2d_pz(E,nu,rho,pz,kds,plane_type)` Creates a plane strain (`plane_type = 0`) or plane stress (`plane_type = 1`) isotropic piezoelectric elasticity element with Young's modulus `E`, Poisson ratio `nu`, mass density `rho`, piezoelectric coefficients(6-by-3), and isotropic dielectric constant `kds`(constant stress) or `kde` (constant strain). A piezoelectric crystal is generally anisotropic but here we have assumed mechanical isotropy.

`PMLElastic2d_pz(Db,rho)` Creates a 2D element with a 5-by-5 piezoelectric elastic property matrix `Db`. Other than the piezoelectric elastic properties, this constructor is identical to the previous one.

`PMLElastic2hd_pz(E,nu,rho,pz,kds)` Creates a plane stress isotropic piezoelectric elasticity element with Young's modulus `E`, Poisson ratio `nu`, mass density `rho`, piezoelectric coefficients(6-by-3), and isotropic dielectric constant `kds`(constant stress) or `kde` (constant strain). A piezoelectric crystal is generally anisotropic but here we have assumed mechanical isotropy. This element is for piezoelectric actuation by an electric field orthogonal to the plane of analysis.

`PMLElastic2hd_pz(Db,rho)` Creates a 2D element with a 4-by-4 piezoelectric elastic property matrix `Db`. Other than the piezoelectric elastic properties, this constructor is identical to the previous one.

`PMLElastic3d_pz(E,nu,rho,pz,kds)` Creates an isotropic 3D piezoelectric elasticity element with Young's modulus `E`, Poisson ratio `nu`, mass density `rho`, piezoelectric coefficients(6-by-3), and isotropic dielectric constant `kds`(constant stress) or `kde` (constant strain). A piezoelectric crystal is generally anisotropic but here we have assumed mechanical isotropy.

`PMLElastic3d_pz(Db,rho)` Creates a 3D element with a 9-by-9 piezoelectric elastic property matrix `Db`. Other than the piezoelectric elastic properties, this constructor is identical to the previous one.

5.6 Electromechanical coupling elements

The `CoupleEM2d` classes implements electromechanical coupling elements. Currently only a 2D implementation is available. The general constructor takes the form,

```
etype = make_material_couple_em(eps,analysistype) Constructs and returns a CoupleEM2d element,
    depending on the given arguments. eps is the material permittivity, and etype which is the element
    type may be either planestrain or planestress.
```

The variable `eps` is the element permittivity. The variable `analysis_type` can take one of the following strings,

- `planestrain`: 2 dimensional planestrain analysis
- `planestress`: 2 dimensional planestress analysis

These elements solve the following equation,

$$0 = \nabla \cdot \mathbf{D} \tag{21}$$

$$\mathbf{D} = \kappa_{d\sigma} \mathbf{E} \tag{22}$$

$$\mathbf{E} = -\nabla \phi \tag{23}$$

on a domain that can deform finitely. This is the only element that implemented that considers finite deformation. This is because the electromechanical coupling is a second order effect and does not arise in linear theory where we assume that the domain does not deform. Here, \mathbf{D} is the electric displacement, \mathbf{E} is the electric field, $\kappa_{d\sigma}$ is the permittivity at constant stress, and ϕ is the voltage potential.

This element alone can not solve the electromechanical problem. It must be overlayed with one of the elastic elements presented in the previous section.

The classes provides the following constructors:

```
CoupleEM2d(kappa) Creates a 2D element with kappa the permittivity at constant stress of the element.
```

5.7 Discrete circuit elements

The `resistor`, `capacitor`, `inductor`, and `VIsrc` classes implement 1D line elements which enable nodal analysis of circuits. The general constructor takes the form,

`etype = make_material_circuit_LRC(mtype,analysistype)` The variable `analysistype` takes a string `resistor`, `capacitor`, `inductor` and constructs the appropriate element. The variable `mtype` defines the numerical value of the component. It can be a real number or a table which contains the real and imaginary part of the number.

`etype = make_material_circuit_wire()` This constructs a short circuit element. By defining the element variables of this element, it can be converted to a voltage or current source.

Used alone, they can solve simple circuits, but the usage in HiQLab is to connect these to mechanical resonator meshes.

Resistor element

The equation governing this element is,

$$\frac{1}{R} (V_1 - V_2) = I \quad (24)$$

and the matrix representation is,

$$\begin{bmatrix} 1/R & -1/R \\ -1/R & 1/R \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (25)$$

The constructors for this element are:

`Resistor(resist)` Creates a 1D lumped resistor element with resistance `resist`.

`Resistor(resist_table)` Creates a 1D lumped resistor element with complex resistance. The value is extracted from the table `resist_table={resist_r,resist_i}` and is given as `(resist_r + iresist_i)`.

Capacitor element

The equation governing this element is,

$$Q = CV \quad (26)$$

$$I = \frac{dQ}{dt} = C \frac{dV}{dt} \quad (27)$$

Since the capacitor is a short circuit, the terms only appear in the first derivative for the matrix formulation.

$$\begin{bmatrix} C & -C \\ -C & C \end{bmatrix} \begin{bmatrix} \dot{V}_1 \\ \dot{V}_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (28)$$

The constructors for this element are:

`Capacitor(cap)` Creates a 1D lumped capacitor element with capacitance `cap`.

`Capacitor(cap_table)` Creates a 1D lumped capacitor element with complex capacitance. The value is extracted from the table `cap_table={cap_r,cap_i}` and is given as `(cap_r + icap_i)`.

Inductor element

The equation governing this element is,

$$V_1 - V_2 = L \frac{dI}{dt} \quad (29)$$

The matrix representation becomes,

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -L \end{bmatrix} \begin{bmatrix} \dot{V}_1 \\ \dot{V}_2 \\ \dot{I}_e \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ I_e \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (30)$$

The constructors for this element are:

Inductor(induct) Creates a 1D lumped inductor element with inductance **induct**.

Inductor(induct_table) Creates a 1D lumped inductor element with complex inductance. The value is extracted from the table **induct_table**={**induct_r**,**induct_i**} and is given as (**induct_r** + *i***induct_i**).

Short circuit, Voltage source, and Current source element

The equation governing this element is,

$$V_1 - V_2 = E \quad (31)$$

The matrix representation becomes,

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ I \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ E \end{bmatrix} \quad (32)$$

where an element variable I which represents the current has been introduced. This element can represent different states by the following procedures.

1. Short circuit(default): Set the value E to zero. Since this is a force boundary condition of zero, it is done by default when the element is constructed.
2. Voltage source: Set the value E to the desired voltage through specifying a force boundary condition of value E on the element variable through the **set_elements_bc** function. (See section on boundary conditions for details).
3. Current source: Set the value I to the desired current through specifying a displacement boundary condition of value I on the element variable through the **set_elements_bc** function. (See section on boundary conditions for details).

The constructors for this element are:

VIsrc() Creates a 1D lumped voltage source, current source, or short circuited wire.

5.8 Electrode

These elements are the key to the coupled resonator circuit analysis available. They serve as an interface element between the discrete circuit elements and finite element meshes. The general constructor takes the form,

`eltnum, index = add_electrode(etype, nodenum, efunc, lt)` The variable `etype` refers to the type of electrode element to be used. Though there are two available, `electrode`, `electrode2`, only support for the first is available. `efunc` must be a global function which ties multiple potential variables of the finite element mesh together to one global variable. `nodenum` refers to the node number of the voltage variable that the global variable is tied together with. The last argument `lt` is optional. In the case of 2D analysis, this variable is used to link the difference between the displacements and force variables which are given per unit normalized length. Thus for the 2D plane stress case, `lt` must equal `layer_thickness/characteritic.length`. The index of this global variable is returned by `index` as well as the element number `eltnum`.

`elt, index = make_material_electrode(etype, efunc, lt)` This constructor conducts the same procedure as above but does not take in the `nodenum`, and thus does not add the electrode element to the mesh. Instead it will just return the global index number `index` and the element `elt`. The user is recommended to use the previous constructor.

A schematic of this electrode is shown in the figure. The equation governing this element is,

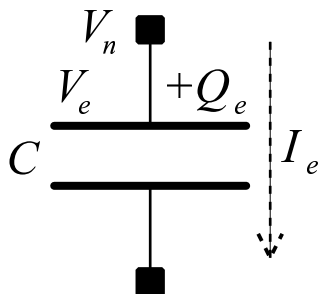


Figure 15: Electrode element

$$Q_e = C_e V_e \quad (33)$$

The matrix representation becomes,

$$\begin{bmatrix} 0 & 0 & \mathbf{lt} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{V}_n \\ \dot{V}_e \\ \dot{Q}_e \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} V_n \\ V_e \\ Q_e \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (34)$$

V_n represents the voltage variable at the node which is linked to the finite element mesh. Two element variables are introduced, V_e and Q_e . V_e , which is additionally a global variable, is introduced to tie the

selected potentials of the finite element mesh to one variable. This global variable is then linked to V_n . Thus a shape function for the global variable must be specified for the formulation. Q_e represents the total charge on the plate.

The classes provides the following constructors:

`Electrode(vglobalid)` Creates an Electrode element with `vglobalid`.

`Electrode2(vglobalid)` Creates an Electrode element with `vglobalid`.

6 Linear material models

The set of linear models in Voigt notation can be expressed by the following equation,

$$\boldsymbol{\varepsilon} = \mathbb{D}_{\mathbf{E},T}\boldsymbol{\sigma} + \mathbf{d}_{\boldsymbol{\sigma},T}\mathbf{E} + \boldsymbol{\alpha}_{\boldsymbol{\sigma},\mathbf{E}}\Delta T \quad (35)$$

$$\mathbf{D} = \mathbf{d}_{\mathbf{E},T}\boldsymbol{\sigma} + \boldsymbol{\kappa}_{\boldsymbol{\sigma},T}\mathbf{E} + \mathbf{p}_{\boldsymbol{\sigma}}\Delta T \quad (36)$$

$$\Delta S = \boldsymbol{\alpha}_{\mathbf{E},T} + \mathbf{p}_{\boldsymbol{\sigma},T}\mathbf{E} + \frac{C_{\boldsymbol{\sigma},\mathbf{E}}}{T}\Delta T \quad (37)$$

or in matrix notation,

$$\begin{bmatrix} \boldsymbol{\varepsilon} \\ \mathbf{D} \\ \Delta S \end{bmatrix} = \begin{bmatrix} \mathbb{D}_{\mathbf{E},T} & \mathbf{d}_{\boldsymbol{\sigma},T} & \boldsymbol{\alpha}_{\boldsymbol{\sigma},\mathbf{E}} \\ \mathbf{d}_{\mathbf{E},T}^T & \boldsymbol{\kappa}_{\boldsymbol{\sigma},T} & \mathbf{p}_{\boldsymbol{\sigma},\mathbf{E}} \\ \boldsymbol{\alpha}_{\mathbf{E},T}^T & \mathbf{p}_{\boldsymbol{\sigma},T}^T & \frac{C_{\boldsymbol{\sigma},\mathbf{E}}}{T} \end{bmatrix} \begin{bmatrix} \boldsymbol{\sigma} \\ \mathbf{E} \\ \Delta T \end{bmatrix} \quad (38)$$

Here, $\boldsymbol{\varepsilon}$ denotes the linearized strain tensor, $\boldsymbol{\sigma}$ the stress tensor, \mathbf{D} the electric displacement, \mathbf{E} the electric field, ΔS the change in entropy, and ΔT the change in temperature. The material dependent coefficients are denoted by, \mathbf{s} the compliance tensor, \mathbf{d} the piezoelectric strain coefficient, $\boldsymbol{\alpha}$ the linear thermal expansion coefficient, $\boldsymbol{\kappa}$ the dielectric coefficient, \mathbf{p} the pyroelectric coefficient, C the heat capacity, and T is the reference temperature. The subscripts denote the fields which are taken as constant in evaluating the coefficients. We assume these coefficients are represented in Voigt notation shown in Table 5. Additionally, the strain tensor in

Table 5: Voigt notation

Voigt	1	2	3	4	5	6
(i, j)	(1,1)	(2,2)	(3,3)	(1,2)	(2,3)	(3,1)

vector form is represented by,

$$\boldsymbol{\varepsilon} = [\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{12}, 2\varepsilon_{23}, 2\varepsilon_{31}]^T \quad (39)$$

Depending on the fields that are coupled, certain portions of the relation above are extracted. Often, instead of the compliance \mathbb{D} , the inverse value representing the stiffness $\mathbb{C} = \mathbb{D}^{-1}$ is used. The number of material constants required to represent the material differ depending on the geometry. These are summarized in Table 6.

Table 6: Material constants for different crystals

Crystal	Elastic(\mathbb{C})	Piezo(\mathbf{d})	Thermal($\boldsymbol{\alpha}$)	Dielectric($\boldsymbol{\kappa}$)	Pyro(\mathbf{p})
Isotropic	$\mathbb{C}_{12}, \mathbb{C}_{44}$	(-)	$\boldsymbol{\alpha}_T$	$\boldsymbol{\kappa}$	(-)
Cubic	$\mathbb{C}_{11}, \mathbb{C}_{12}, \mathbb{C}_{44}$	(-)	$\boldsymbol{\alpha}_T$	$\boldsymbol{\kappa}$	(-)
Hexagonal	$\mathbb{C}_{11}, \mathbb{C}_{12}, \mathbb{C}_{13}, \mathbb{C}_{33}, \mathbb{C}_{55}$	$\mathbf{d}_{16}, \mathbf{d}_{31}, \mathbf{d}_{33}$	$\boldsymbol{\alpha}_{T1}, \boldsymbol{\alpha}_{T2}$	$\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2$	(-)

6.1 Elasticity

For elasticity, only the terms relating stress and strain are extracted. The compliance tensor is inverted to obtain stress in terms of strain as,

$$\boldsymbol{\sigma} = \mathbb{C}\boldsymbol{\varepsilon} \quad (40)$$

$$\mathbb{C} = \mathbb{D}^{-1} \quad (41)$$

The number of elastic constants that must be specified differ depending on the symmetry of the crystal.

6.1.1 Isotropic material

Required parameters in mtype: [E and nu] or [lambda and mu]

Two numbers define the elastic properties of an isotropic material. In matrix form the stiffness is,

$$\mathbb{C}_{\text{isotropic}} = \begin{bmatrix} \mathbb{C}_{12} + 2\mathbb{C}_{44} & \mathbb{C}_{12} & \mathbb{C}_{12} & 0 & 0 & 0 \\ \mathbb{C}_{12} & \mathbb{C}_{12} + 2\mathbb{C}_{44} & \mathbb{C}_{12} & 0 & 0 & 0 \\ \mathbb{C}_{12} & \mathbb{C}_{12} & \mathbb{C}_{12} + 2\mathbb{C}_{44} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{C}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbb{C}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbb{C}_{44} \end{bmatrix} \quad (42)$$

The values \mathbb{C}_{12} and \mathbb{C}_{44} correspond to the Lamé constants λ and μ and are related to the Young's modulus E and Poisson ratio ν by,

$$\mathbb{C}_{12} = \lambda = \frac{\nu E}{(1 - 2\nu)(1 + \nu)} \quad (43)$$

$$\mathbb{C}_{44} = \mu = \frac{E}{2(1 + \nu)} \quad (44)$$

We can express the material tensors in a coordinate free notation where given crystal axes orientation $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$, the elasticity tensor can be expressed as,

$$\mathbb{C}_{\text{cubic}} = \mathbb{C}_{12}\mathbf{1} \otimes \mathbf{1} + 2\mathbb{C}_{44}\mathbb{I}_{\text{sym}}$$

6.1.2 Cubic material

Required parameters in mtype: [alpha, lambda, and mu]

Two numbers define the elastic properties of an isotropic material. In matrix form the stiffness is,

$$\mathbb{C}_{\text{cubic}} = \begin{bmatrix} \mathbb{C}_{11} & \mathbb{C}_{12} & \mathbb{C}_{12} & 0 & 0 & 0 \\ \mathbb{C}_{12} & \mathbb{C}_{11} & \mathbb{C}_{12} & 0 & 0 & 0 \\ \mathbb{C}_{12} & \mathbb{C}_{12} & \mathbb{C}_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{C}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbb{C}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbb{C}_{44} \end{bmatrix} \quad (45)$$

The cubic coefficients are related to the usual expression for cubic materials λ, μ, α by the relations,

$$\begin{aligned}\mathbb{C}_{11} &= \alpha \\ \mathbb{C}_{12} &= \lambda \\ \mathbb{C}_{44} &= \mu\end{aligned}$$

We can express the material tensors in a coordinate free notation where given the cubic coefficients c_{11}, c_{12}, c_{44} and crystal axes orientation $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$, the elasticity tensor can be expressed as,

$$\mathbb{C}_{cubic} = c_{12}\mathbf{1} \otimes \mathbf{1} + 2c_{44}\mathbb{I}_{sym} + (c_{11} - c_{12} - 2c_{44})(\mathbf{a} \otimes \mathbf{a} \otimes \mathbf{a} \otimes \mathbf{a} + \mathbf{b} \otimes \mathbf{b} \otimes \mathbf{b} \otimes \mathbf{b} + \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{c})$$

6.1.3 Hexagonal material

Required parameters in mtype: $[c_{11}, c_{12}, c_{13}, c_{33}, \text{ and } c_{55}]$

The crystal has an in plane hexagonal structure giving it an isotropic property in plane. The material begin piezoelectric has no center of symmetry(inversion center). A hexagonal crystal has the following structure for the elasticity tensor bbC_{hex} , piezoelectric strain coefficients \mathbf{d}_{hex} and dielectric constants $\kappa_{d\sigma}$ in Voigt notation. The 1,2 axes are assumed to be in the isotropic crystal plane with the 3 axis perpendicular to this plane.

$$\mathbb{C}_{hex} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{c_{11}-c_{12}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{55} \end{bmatrix} \quad (46)$$

In a hexagonal material, given the stiffness coefficients, $c_{11}, c_{12}, c_{13}, c_{33}, c_{55}$, the elasticity tensor can be expressed as,

$$\begin{aligned}\mathbb{C}_{hex} &= c_{12}\mathbf{1} \otimes \mathbf{1} + (c_{11} - c_{12})\mathbb{I}_{sym} \\ &+ (c_{33} - c_{11})(\mathbf{c} \otimes \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{c}) \\ &+ (c_{13} - c_{12})(\mathbf{a} \otimes \mathbf{a} \otimes \mathbf{c} \otimes \mathbf{c} + \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{a} \otimes \mathbf{a} + \mathbf{b} \otimes \mathbf{b} \otimes \mathbf{c} \otimes \mathbf{c} + \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{b} \otimes \mathbf{b}) \\ &+ \left(c_{55} - \frac{c_{11} - c_{12}}{2}\right)(\mathbf{b} \otimes \mathbf{c} \otimes \mathbf{b} \otimes \mathbf{c} + \mathbf{b} \otimes \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{b} + \mathbf{c} \otimes \mathbf{b} \otimes \mathbf{b} \otimes \mathbf{c} + \mathbf{c} \otimes \mathbf{b} \otimes \mathbf{c} \otimes \mathbf{b}) \\ &+ \left(c_{55} - \frac{c_{11} - c_{12}}{2}\right)(\mathbf{c} \otimes \mathbf{a} \otimes \mathbf{c} \otimes \mathbf{a} + \mathbf{c} \otimes \mathbf{a} \otimes \mathbf{a} \otimes \mathbf{c} + \mathbf{a} \otimes \mathbf{c} \otimes \mathbf{c} \otimes \mathbf{a} + \mathbf{a} \otimes \mathbf{c} \otimes \mathbf{a} \otimes \mathbf{c})\end{aligned}$$

6.2 Thermoelasticity

For thermoelasticity, the terms relating stress, strain, entropy and temperature are extracted. The compliance tensor is inverted to obtain stress in terms of strain as,

$$\begin{bmatrix} \boldsymbol{\sigma} \\ \Delta S \end{bmatrix} = \begin{bmatrix} \mathbb{C} & -\mathbb{C}\boldsymbol{\alpha} \\ \boldsymbol{\alpha}^T \mathbb{C} & \frac{c}{T} - \boldsymbol{\alpha}^T \mathbb{C} \boldsymbol{\alpha} \end{bmatrix} \begin{bmatrix} \boldsymbol{\varepsilon} \\ \Delta T \end{bmatrix} \quad (47)$$

Additional to this, a constitutive equation must be given for the heat flux \mathbf{q} . Standard linear Fourier model is assumed.

$$\mathbf{q} = \boldsymbol{\kappa}_T \nabla T \quad (48)$$

where, $\boldsymbol{\kappa}_T$ is the conductivity tensor.

6.2.1 Isotropic material

Required parameters in mtype: Parameters for isotropic elastic material plus [at,cp, and kt]

The elasticity tensor takes the form,

$$\mathbb{C} = \mathbb{C}_{\text{isotropic}} \quad (49)$$

The linear thermal coefficient vector becomes,

$$\boldsymbol{\alpha}_T = [\alpha_T, \alpha_T, \alpha_T, 0, 0, 0]^T \quad (50)$$

The conductivity takes the form,

$$\boldsymbol{\kappa}_T = \begin{bmatrix} \kappa_T & 0 & 0 \\ 0 & \kappa_T & 0 \\ 0 & 0 & \kappa_T \end{bmatrix} \quad (51)$$

Two numbers define the elastic properties of an isotropic material. In matrix form the stiffness is,

6.2.2 Cubic material

Required parameters in mtype: Parameters for cubic elastic material plus [at,cp, and kt]

The elasticity tensor takes the form,

$$\mathbb{C} = \mathbb{C}_{\text{cubic}} \quad (52)$$

The linear thermal coefficient vector becomes,

$$\boldsymbol{\alpha}_T = [\alpha_T, \alpha_T, \alpha_T, 0, 0, 0]^T \quad (53)$$

The conductivity takes the form,

$$\boldsymbol{\kappa}_T = \begin{bmatrix} \kappa_T & 0 & 0 \\ 0 & \kappa_T & 0 \\ 0 & 0 & \kappa_T \end{bmatrix} \quad (54)$$

6.3 Piezoelectric elasticity

For piezoelectric elasticity, the terms relating stress, strain, electric displacement and electric field are extracted. The compliance tensor is inverted to obtain stress in terms of strain as,

$$\begin{bmatrix} \boldsymbol{\sigma} \\ \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbb{C} & -\mathbf{C}\mathbf{d} \\ \mathbf{d}^T\mathbb{C} & \boldsymbol{\kappa}_{\sigma,T} - \mathbf{d}^T\mathbb{C}\mathbf{d} \end{bmatrix} \begin{bmatrix} \boldsymbol{\varepsilon} \\ \mathbf{E} \end{bmatrix} \quad (55)$$

6.3.1 Hexagonal material

Required parameters in mtype: Parameters for hexagonal elastic material plus [kds1,kds3,d16,d33 and d31]

The elasticity tensor takes the form,

$$\mathbb{C} = \mathbb{C}_{\text{hexagonal}} \quad (56)$$

The linear piezoelectric coefficient matrix becomes,

$$\mathbf{d} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \mathbf{d}_{16} \\ 0 & 0 & 0 & 0 & \mathbf{d}_{16} & 0 \\ \mathbf{d}_{31} & \mathbf{d}_{31} & \mathbf{d}_{33} & 0 & 0 & 0 \end{bmatrix} \quad (57)$$

The permittivity takes the form,

$$\boldsymbol{\kappa}_T = \begin{bmatrix} \boldsymbol{\kappa}_1 & 0 & 0 \\ 0 & \boldsymbol{\kappa}_1 & 0 \\ 0 & 0 & \boldsymbol{\kappa}_3 \end{bmatrix} \quad (58)$$

6.4 Electrostatics

For an electrostatic problem, the terms relating electric displacement and electric field are extracted.

$$\mathbf{D} = \boldsymbol{\kappa}_{\sigma,T} \mathbf{E} \quad (59)$$

6.4.1 Isotropic material

Required parameters in `mtype`: Parameters for isotropic elastic material plus [`at`, `cp`, and `kt`]

The permittivity takes the form,

$$\boldsymbol{\kappa} = \begin{bmatrix} \boldsymbol{\kappa} & 0 & 0 \\ 0 & \boldsymbol{\kappa} & 0 \\ 0 & 0 & \boldsymbol{\kappa} \end{bmatrix} \quad (60)$$

6.5 Supporting functions

`get_material(mtype)` Converts a material name `mtype` to a table of material properties and returns this table.

`wafer_orientation(wafer, angle)` Computes crystal axes for a cubic material given the wafer orientation `wafer`, either '100' or '111', and the angle [rad] between the global coordinate x-axis and a projection of a material axis onto the x-y plane. A table `axis` containing the two 3-dimensional vectors which define the direction of the x-y axes of the crystal will be returned, components of the `axis1` followed by those of `axis2`.

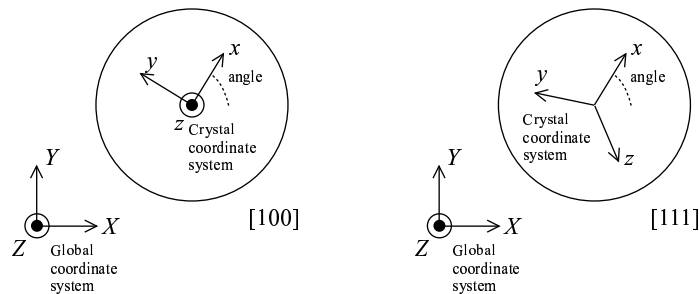


Figure 16: Crystal orientation (wafer and angle)

```
function isotropic_elasticity(mtype, etype, D)
function cubic_elasticity(mtype, etype, axis1, axis2, D)
function hexagonal_elasticity(mtype, etype, axis1, axis2, D)

function isotropic_thermoelasticity(mtype, etype, Db)
function cubic_thermoelasticity(mtype, etype, axis1, axis2, Db)

function piezoelectric_elasticity(mtype, etype, axis1, axis2, Db)
```

7 Non-dimensionalization

The solution to involving coupled fields can cause computational difficulties to the various physical time scales that exist. As a result the magnitude of the entries in the matrices can vary tremendously, leading to very ill-conditioned matrices. To circumvent this problem, non-dimensionalization of dimensional parameters is conducted.

7.1 Incorporating non-dimensionalization

Non-dimensionalization can easily be incorporated in the analysis by specifying the functions summarized in Table 7 at the beginning of the input file immediately after the mesh construction. The only thing that the user must take care is on which functions return dimensionalized values and which do not. Generally, values which are intermediate results are returned in non-dimensionalized form and those that are the final results are dimensionalized. For instance, an array returning just the free degrees of freedom would be non-dimensionalized as opposed to an array of nodal degrees of freedom at every node in the mesh would be dimensionalized. These are summarized in Tables 8 and 9. Thus if values are extracted from the arrays `disp` or `force` obtained from,

```
disp = Mesh_get_disp(mesh);  
force= Mesh_get_force(mesh);
```

they will be in their dimensional form. Also extraction of desired quantities by multiplying `disp` or `force` with the sense vectors obtained from,

```
sense_disp_vec = Mesh_get_sense_disp(mesh,'disp_func');  
sense_force_vec= Mesh_get_sense_force(mesh,'force_func');
```

will also result in dimensional results.

Vectors `U` or `F` obtained through,

```
U = Mesh_get_u(mesh);  
F = Mesh_assemble_k(mesh) * U;
```

will contain only the free dofs in their nondimensional form. But multiplication of these vectors with the sense vectors obtained through,

```
sense_u_vec = Mesh_get_sense_u(mesh,'u_func');  
sense_f_vec = Mesh_get_sense_f(mesh,'f_func');
```

will give dimensional results.

See example of a MEMS cantilever in the Examples manual for details on how to use these functions.

Table 7: Functions to evaluate non-dimensional constants

Function name	Required fields	Key constants	Aux constants
<code>mech_nondim(mtype, cL)</code>	<code>mtype.E</code> , <code>mtype.nu</code> , <code>mtype.rho</code> , <code>cL</code>	M, L, T	F
<code>ted_nondim(mtype, cL)</code>	<code>mtype.E</code> , <code>mtype.nu</code> , <code>mtype.rho</code> , <code>mtype.at</code> , <code>mtype.cp</code> , <code>mtype.kt</code> , (<code>mtype.T0</code> or <code>dim_scales.T0</code>), <code>cL</code>	M, L, T, Th	F, Qt
<code>pz_nondim(mtype, cL)</code>	<code>mtype.E</code> , <code>mtype.nu</code> , <code>mtype.rho</code> , <code>mtype.kds</code> , <code>mtype.d</code> , <code>cL</code>	M, L, T, A	F, V, Q, E, R
<code>em_nondim(mtype, cL, (eps))</code>	<code>mtype.E</code> , <code>mtype.nu</code> , <code>mtype.rho</code> , <code>mtype.kds</code> , <code>mtype.d</code> , <code>cL</code> , (eps or <code>mtype.eps</code> or <code>dim_scales.eps</code>)	M, L, T, A	F, V, Q, E, R

Table 8: Returns dimensional quantities

function name	value returned
<code>Mesh_x.m</code>	A coordinate of a specific node
<code>Mesh_get_x.m</code>	Array of nodal coordinates
<code>Mesh_get_disp.m</code>	Array of nodal displacements
<code>Mesh_get_force.m</code>	Array of nodal forces
<code>Mesh_get_sense_disp.m</code>	Sense vector for nodal displacements
<code>Mesh_get_sense_force.m</code>	Sense vector for nodal forces

Table 9: Returns non-dimensional quantities

function name	value returned
Mesh_get_u.m	Vector of displacement free dofs
Mesh_set_u.m	Set a vector of displacement free dofs
Mesh_assemble_k.m	Assemble stiffness matrix
Mesh_assemble_mk.m	Assemble mass and stiffnes matrices
Mesh_assemble_mkc.m	Assemble mass,stiffness, and damping matrices
Mesh_assemble_dR.m	Assemble gradient of residual
Mesh_assemble_R.m	Assemble residual
Mesh_get_sense_u.m	Sense vector for displacement free dofs
Mesh_get_sense_f.m	Sense vector for force free dofs
Mesh_get_drive_f.m	Drive vector for force free dofs
Mesh_get_sense_globals_u.m	Sense vector for displacement global variable free dofs
Mesh_get_sense_globals_f.m	Sense vector for force global variable free dofs
Mesh_get_sense_globals_f.m	Sense vector for force global variable free dofs
Mesh_get_drive_elements_u.m	Drive vector for displacement element variable free dofs
Mesh_get_sense_elements_f.m	Sense vector for force global variable free dofs
Mesh_get_drive_elements_f.m	Drive vector for force global variable free dofs

7.2 Compute non-dimensionalizing constants

Depending on the fields that are involved, there are currently four functions shown in Table 7 which compute the non-dimensionalizing constants given representative material parameters and geometry. The key constants are, M (mass), L (length), T (time), A (current), and Th (temperature), which are essential in non-dimensionalizing the appropriate fields. The auxiliary constants, F (force), Qt (thermal flux), V (voltage), Q (charge), E (e-field), and R (resistance), are derived from these key constants. Their dimensions are presented in Table 10.

Table 10: Dimensions of auxiliary variables

Variable name	Field name	M	L	T	Th	A
F	force	1	1	-2	-	-
Qt	thermal flux	1	-	-3	-	-
Q	current	-	-	1	-	1
V	voltage	1	2	-3	-	-1
E	e-field	1	1	-3	-	-1
R	resistance	1	2	-3	-	-2

Further details on how these are computed from the material properties are presented below in the codelist.

`mech_nondim(mtype,cL)` Computes characteristic scales (M,L,T) and dimensional quantities (F) from a table of material properties `mtype` and characteristic length scale `cL`, which are used for non-dimensionalization in a mechanical problem. `mtype` must have the fields `rho`(mass density) and `E` (Youngs modulus).

$$\begin{aligned} M &= \rho * cL^3 \\ L &= cL \\ T &= \frac{cL}{\sqrt{E/\rho}} \end{aligned}$$

A table named `dim_scales` with these fields is returned.

`ted_nondim(mtype,cL)` Computes characteristic scales (M,L,T,Th) and dimensional quantities (F,Qt) from a table of material properties `mtype` and characteristic length scale `cL`, which are used for non-dimensionalization in a mechanical problem. `mtype` must have the fields `rho`(mass density) and `E` (Youngs modulus), `at`(linear coefficient of thermal expansion), `cp`(specific heat at constant pressure), and `T0`(ambient temperature).

$$\begin{aligned} M &= \rho * cL^3 \\ L &= cL \\ T &= \frac{cL}{\sqrt{E/\rho}} \\ Th &= \frac{T0 * at * E}{\rho * cp} \end{aligned}$$

A table named `dim_scales` with these fields is returned.

`pz_nondim(mtype, cL)` Computes characteristic scales (M, L, T, A) and dimensional quantities (F, V, Q, E, R) from a table of material properties `mtype` and characteristic length scale `cL`, which are used for non-dimensionalization in a piezoelectric mechanical problem. `mtype` must have the fields `rho` (mass density) and `E` (Youngs modulus), `kds` (permittivity at constant stress), and `d` (piezoelectric strain coefficients).

$$\begin{aligned} M &= \rho * cL^3 \\ L &= cL \\ T &= \frac{cL}{\sqrt{E/\rho}} \\ A &= \frac{kds * cL^2}{d * T} \end{aligned}$$

A table named `dim_scales` with these fields is returned.

`em_nondim(mtype, cL, (eps))` Computes characteristic scales (M, L, T, A) and dimensional quantities (F, V, Q, E, R) from a table of material properties `mtype` and characteristic length scale `cL`, which are used for non-dimensionalization in an electromechanical problem. `mtype` must have the fields `rho` (mass density) and `E` (Youngs modulus), and `eps` (permittivity at constant stress).

$$\begin{aligned} M &= \rho * cL^3 \\ L &= cL \\ T &= \frac{cL}{\sqrt{E/\rho}} \\ A &= \frac{eps * E * cL^3}{T} \end{aligned}$$

7.3 Non-dimensionalize material parameters

`material_normalize(ftype, ...)` Non-dimensionalizes all arguments ... by the the dimensional scale `dim_scales[ftype]`. `ftype` must be a string corresponding to a characteristic scale (M, L, T, Th, A) or a dimensional quantity $F, V, Q, E, R, Qt, etc.$ that has been predefined in the table `dim_scales`. If such a field does not exist, `dim_scales[ftype]` is assumed one. The number of input arguments will be returned.

`mech_material_normalize(m)` Non-dimensionalizes the mechanical fields of the material `m` given as a table by the characteristic scales defined in `dim_scales`, and returns a table with ONLY these mechanical fields. There is no restriction on the fields existing in `m`, but only the fields, `rho`, `E`, `lambda`, `mu`, `alpha`, `c11`, `c12`, `c13`, `c33`, `c55` will be non-dimensionalized. If a field in `dim_scales` does not exist, it will be assumed one.

`ted_material_normalize(m)` Non-dimensionalizes the thermomechanical fields of the material `m` given as a table by the characteristic scales defined in `dim_scales`, and returns a table with ONLY these thermomechanical fields. There is no restriction on the fields existing in `m`, but only the fields, `rho`, `E`, `lambda`, `mu`, `alpha`, `at`, `cp`, `kt`, `T0` will be non-dimensionalized. If a field in `dim_scales` does not exist, it will be assumed one.

`pz_material_normalize(m)` Non-dimensionalizes the piezoelectric-mechanical fields of the material `m` given as a table by the characteristic scales defined in `dim_scales`, and returns a table with ONLY these piezoelectric-mechanical fields. There is no restriction on the fields existing in `m`, but only the fields, `rho`, `c11`, `c12`, `c13`, `c33`, `c55`, `d16`, `d31`, `d33`, `kds1`, `kds3` will be non-dimensionalized. If a field in `dim_scales` does not exist, it will be assumed one.

8 Basic functions (Matlab)

8.1 Loading and deleting Lua mesh input files

The Lua object interface is used in the MATLAB `Mesh_load` function:

`Mesh_load(filename,p)` Creates a Lua interpreter and executes the named file in order to generate a mesh object (which is returned). The mesh should be named “mesh”; if such an object is undefined on output, `Mesh_load` returns an error message. Before executing the named file, `Mesh_load` copies the entries of the structure `p`, which may only be strings or doubles, into the Lua global state; in this way, it is possible to vary mesh parameters from MATLAB.

`Mesh_delete(mesh)` Deletes the mesh object.

8.2 Getting Scaling parameters

`scale_param = Mesh_get_scale(scale_name)` Get a characteristic scale described by the given name.

`[cu,cf] = Mesh_get_scales(mesh)` Return an array of dimensional scales for the problem.

Outputs:

`cu` - scales for the primary variables

`cf` - scales for the secondary (flux) variables

8.3 Obtain basic information about mesh

`ndm = Mesh_get_ndm(mesh)` Return the dimension of the ambient space for the mesh.

`numnp = Mesh_numnp(mesh)` Return the number of nodal points in the mesh.

`ndf = Mesh_get_ndf(mesh)` Return the number of degrees of freedom per node in the mesh.

`numid = Mesh_get_numid(mesh)` Return the total number of degrees of freedom in the mesh.

`numelt = Mesh_numelt(mesh)` Return the number of elements in the mesh.

`nen = Mesh_get_nen(mesh)` Return the maximum number of nodes per element.

`numglobals = Mesh_numglobals(mesh)` Return the number of global degrees of freedom in the mesh

`nbranch_id = Mesh_nbranch_id(mesh)` Return the number of branch variables in the mesh

`x = Mesh_get_x(mesh, (cL))` Return an `ndm`-by-`numnp` array of node positions.

Inputs:

`cL` - characteristic length used for redimensionalization
(default: mesh 'L' scale)

`e = Mesh_get_e(mesh)` Return the element connectivity array (a `maxnen`-by-`numelt` array).

`id = Mesh_get_id(mesh)` Return the variable-to-identifier mapping (a maxndf-by-numnp array). Nodal variables subject to displacement BCs are represented by a 0.

`bc = Mesh_get_bc(mesh)` Return an ndf-by-numnp array of boundary codes. The codes are

- 0 - No boundary condition for this dof
- 1 - Displacement (essential) boundary conditions
- 2 - Flux (natural) boundary conditions

`[p,e,id,bc,numnp] = Mesh_get_parameters(mesh,(cL))` Input:
 cL - characteristic length to redim node positions
 (default: mesh 'L' parameter)
 Return mesh parameters:
 p - Node position array
 e - Element connectivity array (nen-by-numelt)
 id - Variable identifier array (ndf-by-numnp)
 bc - Boundary condition codes (see Mesh_get_bc)
 numnp - Number of nodal points

8.4 Obtain particular information about ids

`ix = Mesh_ix(mesh,i,j)` Return the ith node of element j

`id = Mesh_id(mesh,i,j)` Return the ith variable of node j

`id = Mesh_branchid(mesh,i,j)` Return the ith variable of branch j

`id = Mesh_globalid(mesh,j)` Return the id for jth global variable

`nbranch_id = Mesh_nbranch_id(mesh,j)` Return the number of variables of branch j

8.5 Obtain particular information about id, nodes, or elements

`x = Mesh_x(mesh,i,j,(cL))` Return the ith coordinate of node j.

Inputs:
 i - coordinate index
 j - node number
 cL - characteristic length scale for redimensionalization
 (default: mesh 'L' scale)

`nen = Mesh_get_nen_elt(mesh,j)` Return the number of nodes for element j

8.6 Getting displacements and force

`[u] = Mesh_get_disp(mesh,is_dim)` Get the node displacement array (dimensionless)

Inputs:
 - is_dim - should the vector be redimensionalized? (default: 1)

8.8 Other useful functions

`E = Mesh_mean_power(mesh)` Compute the time-averaged energy flux at each node. TODO: The flux is currently in dimensionless form, but it probably shouldn't be.

`f = Mesh_get_lua_fields(mesh, name, nfields)` Return an array of field values.

Inputs:

`name` - the name of the Lua function to define the fields
`nfields` - number of fields requested

`Mesh_make_harmonic(mesh, omega)` Set $v = i \cdot \omega \cdot u$ and $a = -\omega^2 \cdot u$

Input:

`omega` - forcing frequency
`units` - specify units of forcing frequency (default 'rs'):
 'hz': omega is in units of Hz
 'rs': omega is in units of rad/s
 'nd': omega is in dimensionless units
`cT` : nondimensionalize omega using the given characteristic time

8.9 Assigning and reassigning ids

`int = Mesh_assign_ids(mesh)` Number the degrees of freedom in the mesh. Returns the total number of dofs.

`int = ted_block_mesh(mesh)` Relabel the nodal degrees of freedom so that all mechanical degrees of freedom come first, followed by all thermal degrees of freedom. Return the total number of mechanical degrees of freedom.

`int = pz_block_mesh(mesh)` Relabel the nodal degrees of freedom so that all mechanical degrees of freedom come first, followed by all potential degrees of freedom. Return the total number of mechanical degrees of freedom.

8.10 Producing forcing and sensing pattern vectors

`u = Mesh_get_sense_u(mesh, name, is_reduced)` Return a vector for a displacement sense pattern. The vector is in dimensionless form.

Inputs:

`name` - the name of the Lua function to define the pattern
`is_reduced` - do we want the reduced (vs full) vector? Default: 1

`u = Mesh_get_sense_disp(mesh, name, is_reduced)` Return a vector for a displacement sense pattern. The vector is in dimension form.

Inputs:

`name` - the name of the Lua function to define the pattern
`is_reduced` - do we want the reduced (vs full) vector? Default: 1

`f = Mesh_get_sense_f(mesh, name, is_reduced)` Return a vector for a force sense pattern The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern
is_reduced - do we want the reduced (vs full) vector? Default: 1

`f = Mesh_get_drive_f(mesh, name, is_reduced)` Return a vector for a drive sense pattern The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern
is_reduced - do we want the reduced (vs full) vector? Default: 1

`f = Mesh_get_sense_force(mesh, name, is_reduced)` Return a vector for a force sense pattern The vector is in dimension form.

Inputs:

name - the name of the Lua function to define the pattern
is_reduced - do we want the reduced (vs full) vector? Default: 1

`u = Mesh_get_sense_globals_u(mesh, name)` Return a vector for a global variable displacement sense pattern. The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern

`f = Mesh_get_sense_globals_f(mesh, name)` Return a vector for a global variable force sense pattern. The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern

`f = Mesh_get_drive_globals_f(mesh, name)` Return a vector for a global variable force drive pattern. The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern

`u = Mesh_get_sense_elements_u(mesh, name)` Return a vector for an element variable displacement sense pattern. The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern

`f = Mesh_get_sense_elements_f(mesh, name)` Return a vector for an element variable force sense pattern. The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern

`f = Mesh_get_drive_elements_f(mesh, name)` Return a vector for an element variable force drive pattern. The vector is in dimensionless form.

Inputs:

name - the name of the Lua function to define the pattern

8.11 Getting and setting variables in the Lua environment

`Lua_set_string(L, string_name, string_value)` Set a string variable in the Lua environment

L - the Lua interpreter object
 string_name - the name of the Lua variable (must be string)
 s - a string value (must be string)

`string = Lua_get_string(L, string_name)` Get a string variable out of the Lua environment

L - the Lua interpreter object.
 name - the name of the Lua variable.

Returns an empty string if no such variable exists.

`Lua_set_double(L, double_name, double_value)` Set a numeric variable in the Lua environment

L - the Lua interpreter object
 name - the name of the Lua variable
 x - a number

`[x] = Lua_get_double(L, name)` Get a numeric variable out of the Lua environment

x - the value of the Lua variable

`Lua_set_table_double(L, table_name, double_name, double_value x)` Set a numeric variable in a table in the Lua environment

L - the Lua interpreter object
 table_name - the name of the Lua table
 double_name - the name of the Lua key
 double_value - a number

key can be a number or a string.

`[x] = Lua_get_table_double(L, table_name, double_name)` Get a numeric variable out of a table in the Lua environment

`x` - the value of the Lua variable

key can be a number or a string.

`Lua_set_table_string(L, table_name, string_name, string_value)` Set a string variable in a table in the Lua environment

`L` - the Lua interpreter object
`table_name` - the name of the Lua table
`string_name` - the name of the Lua key
`string_value` - a number

key can be a number or a string.

`[s] = Lua_get_table_string(L, table_name, string_name)` Get a string variable out of a table in the Lua environment

`s` - the string value of the Lua variable

key can be a number or a string.

`Lua_set_array(L, a_name, array, a_type)` Set a matrix variable in the Lua environment

Input:

`L` - the Lua interpreter object
`a_name` - the name of the matrix variable
`array` - a numeric array
`a_type(0)` - the type of array to construct
 0: Real array
 1: Real array of twice the size
 (Not supported yet)
 2: Complex array

`[m_Object] = Lua_get_array(L, name)` Get a matrix variable from the Lua environment

Input:

`L` - the Lua interpreter object
`name` - the name of the Lua variable

8.12 Manipulating the Lua environment

The same interfaces that are automatically bound to Lua are also automatically bound to MATLAB. In addition, several methods are defined which allow MATLAB to manipulate a Lua interpreter:

`Lua_open` Return a pointer to a new Lua interpreter `L`

`Lua_close(L)` Close the Lua interpreter

`Lua_dofile(L,filename)` Execute a Lua file

`Lua_set_mesh(L,name,mesh)` Assign a mesh object to a Lua global

`Lua_get_mesh(L,name)` Retrieve a mesh object from a Lua global

9 Functions for analysis(MATLAB)

9.1 Static analysis

Solves for the static state of a device. The equation,

$$\mathbf{R}(\mathbf{U}) = 0 \quad (61)$$

for the general case, and

$$\mathbf{K}\mathbf{U} = \mathbf{F} \quad (62)$$

for the linear case is solved.

`static_state(mesh,opt)` Solves for the static state. If the field nonlinear is not specified only 1 iteration will be conducted.

```

Input: mesh - Mesh object
*opt
  nonlinear('NR')- Conduct non-linear solve
                  'NR' :Newton-Raphson
                  'MNR':Modified-Newton-Raphson
  kmax(20)       - Max number of iterations
  du_tol(1e-15) - Tolerance for convergence
                  for increment
  R_tol (1e-15) - Tolerance for convergence
                  for residual
  U              - Initial starting vector for solve

```

9.2 Time-harmonic analysis

Solves for the time harmonic state.

$$(\mathbf{K} + i\omega\mathbf{C} - \omega^2\mathbf{M}) \mathbf{u} = \mathbf{F} \quad (63)$$

`harmonic_state(mesh,F,w,opt)` Solves for the time-harmonic state.

```

Input: mesh      - Mesh object
      F          - Forcing vector(in nondimensional form)
      w          - Forcing frequency
*opt
  mkc(0)         - Include damping matrix
  kmax(1)        - Max number of iterations
  du_tol(1e-15) - Tolerance for convergence
                  for increment
  R_tol(1e-15)  - Tolerance for convergence
                  for residual

```

9.3 Modal analysis

The MATLAB sparse eigensolver routine `eigs` is actually an interface to ARPACK (see Section ??). We express all frequencies in radians/s rather than Hertz. We provide one function to compute complex frequencies and associated mode shapes for PML eigenvalue problems:

`[V,w,Q] = pml_mode(M,K,w0,nmodes,opt)` Find the requested number of modes closest in frequency to `w0`. Return an array of mode shapes, a vector of complex frequencies, and a vector of `Q` values. Options are

`use_matlab` Use MATLAB's `eigs` rather than ARPACK? (default: false)
`use_umfpack` Use UMFPACK with MATLAB `eigs`, if present? (default: true)
`disp` Verbosity level? (default: 0)

`[V,w,Q] = tedmode(mesh, w0, nev, opt)` Computes the eigenfrequencies and modes of a thermoelastic problem.

Compute `nev` complex frequencies `w` (in rad/s) near target frequency `w0`, and also associated `Q` values. `V` contains the eigenvectors (mechanical and thermal parts).

Note: `tedmode` will reorder the degrees of freedom in the mesh.

`opt` contains optional parameters:
`mech` - Conduct purely mechanical analysis
`type` - Use a perturbation method ('pert') or linearization ('full'). Default is 'full'.
`T0` - Baseline temperature for use in symmetric linearization
`cT` - Characteristic time scale for redimensionalization (Default: `Mesh_get_scale('T')`)
`use_matlab` - use matlab `eigs` or not (Default:0)

`[V,w,Q] = emmode(mesh, w0, nev, opt)` Computes the eigenfrequencies and modes of an electromechanical problem.

Compute `nev` complex frequencies `w` (in rad/s) near target frequency `w0`, and also associated `Q` values. `V` contains the eigenvectors

`opt` contains optional parameters:
`mech` - Conduct purely mechanical analysis
`type` - Use a perturbation method ('pert') or linearization ('full'). Default is 'full'.
`cT` - Characteristic time scale for redimensionalization (Default: `Mesh_get_scale('T')`)
`use_matlab` - use matlab `eigs` or not (Default:1)

idg_m - array of global numbers for mechanical variables
idg_p - array of global numbers for potential variables

[V,w,Q] = emcmode(mesh, w0, nev, opt) Computes the eigenfrequencies and modes of a electromechanical problem with surrounding circuitry.

Compute nev complex frequencies w (in rad/s) near target frequency w0, and also associated Q values. V contains the eigenvectors

opt must contain following parameters

eno - array of element numbers for electrodes
idg - array of global number for driving electrode

opt contains optional parameters:

mech - Conduct purely mechanical analysis
type - Use a perturbation method ('pert') or linearization ('full'). Default is 'full'.
cT - Characteristic time scale for redimensionalization (Default: Mesh_get_scale('T'))
use_matlab - use matlab eigs or not (Default:1)

9.4 Transfer function evaluation

`[H,freq] = second_order_bode(mesh,wc,drive_pat,sense_pat,opt)` Computes the transfer function given the driving pattern and sensing pattern. The frequency range is set by specifying the center frequency `wc` and the range. Model reduction can be conducted by specifying the number of iterations `kmax` conducted to produce the reduced order model. Different projection bases can also be selected.

```

Output: freq          - Frequency array [rad/s]
        H             - Output
Input:  mesh          - the mesh input
        wc            - center frequency[rad/s]
        drive_pat     - Driving pattern vector
        sense_pat     - Sensing pattern vector
*opt
-freq          - Predefined array of freq
-mkc(0)        - Include damping or not
-cT            - Characteristic time scale for
                redimensionalization
                (Default: Mesh_get_scale('T'))
-wr_min(0.90)  - left  value mag of bode plot
-wr_max(1.10)  - right value mag of bode plot
-w_ndiv(50)    - number divisions in bode plot
-w_type('lin') - division type (linspace or logspace)
-kmax(0)       - number of arnoldi iterations
-realbasis(0)  - use real basis??
-structurep(0) - use structure preserving basis??
-use_umfpack   - use UMFPACK?? (Default: use if exist)

```

If `kmax` and `wc` are given, use model reduction via an Arnoldi expansion about the shift `w0`.

9.5 Model reduction

There is currently one model reduction routine in the MATLAB support files for HiQLab. As before, all frequencies are expressed in radians/s rather than Hz.

`[Mk,Dk,Kk,Lk,Bk,Vk] = rom_arnoldi(M,K,l,b,kk,w0,opt)` Takes `kk` steps of shift-and-invert Arnoldi to form a basis for the Krylov subspace $\mathcal{K}_k((K - (2\pi\omega_0)^2M)^{-1}M, b)$ in order to form a reduced system to estimate the system transfer function. Returns reduced matrices M_k , K_k , l_k , and b_k , along with the projection basis V_k . If `opt.realbasis` is set to true (default is false), then the projection will use a real basis for the span of $[\text{Re}(V_k), \text{Im}(V_k)]$. To do this, the matrix $[\text{Re}(V_k), \text{Im}(V_k)]$ will be orthonormalized using an SVD, and vectors corresponding to values less than `opt.realtol` (default 10^{-8}) will be dropped.

`[Mk,Dk,Kk,Lk,Bk,Vk] = rom_soar(M,D,K,L,B,kk,w0,opt)` Takes `kk` steps of shift-and-invert SOAR to form a basis for the second order Krylov subspace, in order to form a reduced system to estimate the system transfer function. Returns reduced matrices M_k , K_k , l_k , and b_k , along with the projection

basis V_k . If `opt.realbasis` is set to true (default is false), then the projection will use a real basis for the span of $[\text{Re}(V_k), \text{Im}(V_k)]$. To do this, the matrix $[\text{Re}(V_k), \text{Im}(V_k)]$ will be orthonormalized using an SVD, and vectors corresponding to values less than `opt.realtol` (default 10^{-8}) will be dropped. To form the structure preserving base for the thermoelastic problem, the `id` array must be reordered so that the mechanical dofs come first before the thermal dofs. `opt.structurep` must be set to 1, and the number of mechanical degrees of freedom must also be specified.

10 Basic analysis (Lua)

10.1 Functions to obtain basic information about mesh

`ndm = Mesh:get_ndm()` Return the dimension of the ambient space for the mesh.

`numnp = Mesh:numnp()` Return the number of nodal points in the mesh.

`ndf = Mesh:get_ndf()` Return the number of degrees of freedom per node in the mesh.

`numid = Mesh:get_numid()` Return the total number of degrees of freedom in the mesh.

`numelt = Mesh:numelt()` Return the number of elements in the mesh.

`nen = Mesh:get_nen()` Return the maximum number of nodes per element.

`numglobals = Mesh:numglobals()` Return the number of global degrees of freedom in the mesh

`nbranch_id = Mesh:nbranch_id()` Return the number of branch variables in the mesh

10.2 Obtain particular information about ids

`id = Mesh:id(mesh,i,j)` Return the *i*th variable of node *j*

`id = Mesh:branchid(mesh,i,j)` Return the *i*th variable of branch *j*

`id = Mesh:globalid(mesh,j)` Return the id for *j*th global variable

`nbranch_id = Mesh:nbranch_id(mesh,j)` Return the number of variables of branch *j*

11 Plotting results (Matlab)

11.1 Mesh plots

There are several plotting routines for viewing the behavior of 2D meshes:

`plotmesh(mesh,opt)` Plots a given mesh. Options are

- `anchors` Marker for nodes with displacement BC (default: 'g+')
- `forces` Marker for nodes with force BC (default: 'r+')
- `deform` Deform mesh according to first to fields of u ? (default: false)
- `clf` Clear the figure before display? (default: true)
- `axequal` Use equal axes in plots? (default: false)

11.2 Plotting the deformed mesh

`plotfield1d(mesh,opt)` Colors are chosen according to the magnitudes of the u components.

- `ufields` Fields to use for displacement (default: [1])
- `cfields` Fields to use for coloring (default: [1])
- `ncfields` Number of color Fields to obtain
- `axequal` Use equal axes in plots? (default: false)
- `subplot` Subplot setup (default: [length(ncfields), 1])
- `deform` Deform mesh according to first to fields of u ? (default: false)
- `clf` Clear the figure before display? (default: true)
- `axis` Set axes
- `subplot` Subplot size (default is [ncfields 1])
- `xscale` Amount to scale by (for unit change)(Default:1)
- `xlabel` X label (Default: [])
- `ylabel` Y label (Default: [])
- `titles` Title (can be a cell array of titles)(Default: [])

`plotfield2d(mesh,opt)` Colors are chosen according to the magnitudes of the u components.

- `ufields` Fields to use for displacement (default: [1,2])
- `cfields` Fields to use for coloring (default: [1,2])
- `ncfields` Number of color Fields to obtain(default:1)
- `cbias` Bias of the color scale (cmax/cbias-;red)(default: 3)
- `cbar` Add colorbar (Default: false)
- `cscale` Scale field colors together? (Default: false)
- `axequal` Use equal axes in plots? (default: false)

subplot Subplot setup (default: `[length(nfields), 1]`)
deform Deform mesh according to first to fields of u ? (default: false)
clf Clear the figure before display? (default: true)
axis Set axes
subplot Subplot size (default is `[nfields 1]`)
xscale Amount to scale by (for unit change)(Default:1)
xlabel X label (Default: [])
ylabel Y label (Default: [])
titles Title (can be a cell array of titles)(Default: [])

11.3 Animations

plotcycle1d(mesh,s,opt) Plot an animation of the motion of the mesh. The amplitude of motion is scaled by the factor s (which defaults to one if it is not provided). The frames can be written to disk as a sequence of PNG files to make a movie later. The following options can be set through the `opt` structure

framepng Format string for movie frame files (default: [])
nframes Number of frames to be plotted (default: 32)
fpcycle Frames per cycle (default: 16)
startf Start frame number (default: 1)
fpause Pause between re-plotting frames (default: 0.25)
axequal Use equal axes in plots? (default: false)
axis Set axes
subplot Subplot size (default is `[nfields 1]`)
xscale Amount to scale by (for unit change)(Default:1)
xlabel X label (Default: [])
ylabel Y label (Default: [])
titles Title (can be a cell array of titles)(Default: [])
avi_file Title of avi file to generate(Default: []) (Default: NO AVI FILE IS PRODUCED)
avi_w Width of the window size(Default: 300)
avi_h Height of the window size(Default: 300)
avi_left Window distance from left side of monitor(Default: 10)
avi_bottom Window distance from bottom of monitor(Default: def) (Default is set so window touches top of monitor)

plotcycle2d(mesh,s,opt) Plot an animation of the motion of the mesh. The amplitude of motion is scaled by the factor s (which defaults to one if it is not provided). The frames can be written to disk as a sequence of PNG files to make a movie later. The following options can be set through the `opt` structure

framepng Format string for movie frame files (default: [])
nframes Number of frames to be plotted (default: 32)
fpcycle Frames per cycle (default: 16)
startf Start frame number (default: 1)
fpause Pause between re-plotting frames (default: 0.25)
cyscale Color all fields on the same scale? (default: false)
cbias Bias of the color scale (cmax/cbias- γ red)(default: 3)
ufields Fields to use for displacement (default: [1 2])
cfields Fields to use for coloring (default: [1 2])
axequal Use equal axes in plots? (default: false)
subplot Subplot setup (default: [length(cfields), 1])
axis Set axes
subplot Subplot size (default is [nfields 1])
xscale Amount to scale by (for unit change)(Default:1)
xlabel X label (Default: [])
ylabel Y label (Default: [])
titles Title (can be a cell array of titles)(Default: [])
avi_file Title of avi file to generate(Default: []) (Default: NO AVI FILE IS PRODUCED)
avi_w Width of the window size(Default: 300)
avi_h Height of the window size(Default: 300)
avi_left Window distance from left side of monitor(Default: 10)
avi_bottom Window distance from bottom of monitor(Default: def) (Default is set so window touches top of monitor)

11.4 Plotting Bode plots

In addition, there is a function for viewing Bode plots:

plot_bode(freq,H,opt) Plots a Bode plot. **H** is the transfer function evaluated at frequency points **freq**. The option structure **opt** may contain the following options:

usehz Assume **freq** is in Hz (default: false)
logf Use a log scale on the frequency axis (default: false)
magnitude Plot magnitude only (default: false)
visualQ Visually compute Q for the highest peak (default: false)
lstyle Set the line style for the plot (default: 'b')

For example, to plot a reduced model Bode plot on top of an exact Bode plot, we might use the following code:

```
figure(1); hold on
opt.logf = 1;
opt.lstyle = 'b' ; plot_bode(freq_full, H_full, opt);
opt.lstyle = 'r:.'; plot_bode(freq_rom, H_rom, opt);
hold off
```

It is also possible to simultaneously show a deformed mesh and a Bode plot with a marker indicating the excitation frequency.

`plotmesh.bode(mesh,f,H,fcurent,opt)` Plot the deformed mesh and create a Bode plot. The `opt` field is passed through to `plotmesh`.