esys User's Guide: Solving Partial Differential Equations with Escript and Finley

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Lutz Gross *et al.* (Editor)

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Earth Systems Science Computational Centre (ESSCC)
The University of Queensland
Brisbane, Australia
Email: esys@esscc.uq.edu.au

Abstract

`esys.escript` is a python-based environment for implementing mathematical models, in particular those based on coupled, non-linear, time-dependent partial differential equations.

It consists of four major components

- `esys.escript` core library
- finite element solver `esys.finley` (which uses fast vendor-supplied solvers or our paso linear solver library)
- the meshing interface `esys.pycad`
- VTK visualization interface `esys.pyvisi`
- model library modellib

The current version supports parallelization through both MPI for distributed memory and OpenMP for distributed shared memory.

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CHAPTER

ONE

Installation

We offer binary distributions for some systems and source code distributions for others. The binary distributions include Escript/Finley itself and all required packages. The required third-party software packages are included in compliance with their copyrights.

Complete information is available at https://shake200.esscc.uq.edu.au/twiki/bin/view/ESSCC/EsysInstallationGuide.

Please direct any questions you might have to mailto:esys@esscc.uq.edu.au.

CHAPTER

TWO

Tutorial: Solving PDEs

2.1 The First Steps

In this chapter we give an introduction how to use `esys.escript` to solve a partial differential equation (PDE). We assume you are at least a little familiar with Python. The knowledge presented at the Python tutorial at http://docs.python.org/tut/tut.html is more than sufficient.

The PDE we wish to solve is the Poisson equation

$$-\Delta u = f \tag{2.1}$$

for the solution u. The function f is the given right hand side. The domain of interest, denoted by Ω, is the unit square

$$\Omega = [0,1]^2 = \{(x_0;x_1) | 0 \le x_0 \le 1 \text{ and } 0 \le x_1 \le 1\} \tag{2.2}$$

The domain is shown in Figure 2.1.

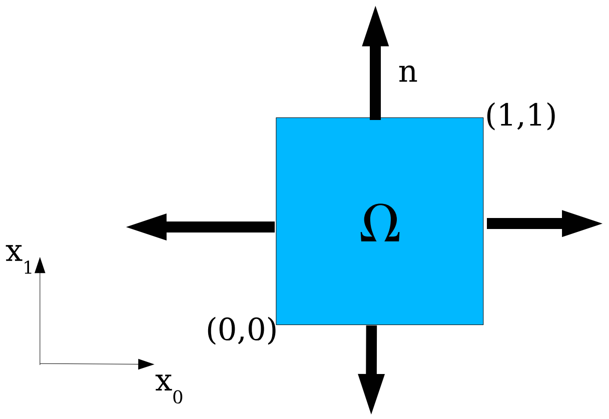


FIGURE 2.1: Domain $\Omega = [0,1]^2$ with outer normal field n.

Δ denotes the Laplace operator, which is defined by

$$\Delta u = (u_{,0})_{,0} + (u_{,1})_{,1} \tag{2.3}$$

where, for any function u and any direction i, $u_{,i}$ denotes the partial derivative of u with respect to i. [1] Basically, in the subindex of a function, any index to the left of the comma denotes a spatial derivative with respect to the

[1]You may be more familiar with the Laplace operator being written as ∇^2, and written in the form

$$\nabla^2 u = \nabla^t \cdot \nabla u = \frac{\partial^2 u}{\partial x_0^2} + \frac{\partial^2 u}{\partial x_1^2}$$

and Equation (2.1) as

$$-\nabla^2 u = f$$

index. To get a more compact form we will write $u_{,ij} = (u_{,i})_{,j}$ which leads to

$$\Delta u = u_{,00} + u_{,11} = \sum_{i=0}^{2} u_{,ii} \tag{2.4}$$

We often find that use of nested $\sum$ symbols makes formulas cumbersome, and we use the more convenient Einstein summation convention . This drops the $\sum$ sign and assumes that a summation is performed over any repeated index. For instance we write

$$x_i y_i = \sum_{i=0}^{2} x_i y_i \tag{2.5}$$

$$x_i u_{,i} = \sum_{i=0}^{2} x_i u_{,i} \tag{2.6}$$

$$u_{,ii} = \sum_{i=0}^{2} u_{,ii} \tag{2.7}$$

$$x_{ij} u_{i,j} = \sum_{j=0}^{2} \sum_{i=0}^{2} x_{ij} u_{i,j} \tag{2.8}$$

$$\tag{2.9}$$

With the summation convention we can write the Poisson equation as

$$-u_{,ii} = 1 \tag{2.10}$$

where $f = 1$ in this example.

On the boundary of the domain Ω the normal derivative $n_i u_{,i}$ of the solution u shall be zero, ie. u shall fulfill the homogeneous Neumann boundary condition

$$n_i u_{,i} = 0\ . \tag{2.11}$$

$n = (n_i)$ denotes the outer normal field of the domain, see Figure 2.1. Remember that we are applying the Einstein summation convention , i.e $n_i u_{,i} = n_0 u_{,0} + n_1 u_{,1}$. [2] The Neumann boundary condition of Equation (2.11) should be fulfilled on the set Γ^N which is the top and right edge of the domain:

$$\Gamma^N = \{(x_0; x_1) \in \Omega | x_0 = 1 \text{ or } x_1 = 1\} \tag{2.12}$$

On the bottom and the left edge of the domain which is defined as

$$\Gamma^D = \{(x_0; x_1) \in \Omega | x_0 = 0 \text{ or } x_1 = 0\} \tag{2.13}$$

the solution shall be identically zero:

$$u = 0\ . \tag{2.14}$$

This kind of boundary condition is called a homogeneous Dirichlet boundary condition . The partial differential equation in Equation (2.10) together with the Neumann boundary condition Equation (2.11) and Dirichlet boundary condition in Equation (2.14) form a so called boundary value problem (BVP) for the unknown function u.

In general the BVP cannot be solved analytically and numerical methods have to be used construct an approximation of the solution u. Here we will use the finite element method (FEM). The basic idea is to fill the domain with a set of points called nodes. The solution is approximated by its values on the nodes. Moreover, the domain is subdivided into smaller sub-domains called elements . On each element the solution is represented by a polynomial of a certain degree through its values at the nodes located in the element. The nodes and its connection through elements is called a mesh. Figure 2.2 shows an example of a FEM mesh with four elements in the $x0$ and four elements in the $x1$ direction over the unit square. For more details we refer the reader to the literature, for instance Reference [18, 8].

`esys.escript` provides the class `Poisson` to define a Poisson equation . (We will discuss a more general form of a PDE that can be defined through the `LinearPDE` class later). The instantiation of a `Poisson` class object requires the specification of the domain Ω. In `esys.escript` the `Domain` class objects are used to describe the geometry of a domain but it also contains information about the discretization methods and the actual solver which is used to solve the PDE. Here we are using the FEM library `esys.finley` . The following statements create the `Domain` object *mydomain* from the `esys.finley` method `Rectangle`

[2]Some readers may familiar with the notation $\frac{\partial u}{\partial n} = n_i u_{,i}$ for the normal derivative.

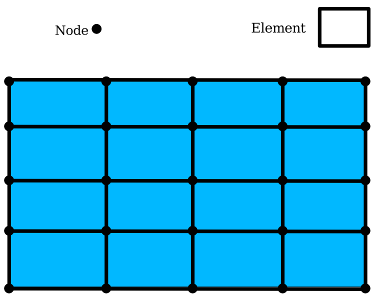


FIGURE 2.2: Mesh of 4 elements on a rectangular domain. Here each element is a quadrilateral and described by four nodes, namely the corner points. The solution is interpolated by a bi-linear polynomial.

```
from esys.finley import Rectangle
mydomain = Rectangle(l0=1.,l1=1.,n0=40, n1=20)
```

In this case the domain is a rectangle with the lower, left corner at point $(0, 0)$ and the right, upper corner at $(l0, l1) = (1, 1)$. The arguments *n0* and *n1* define the number of elements in x_0 and x_1-direction respectively. For more details on `Rectangle` and other `Domain` generators within the `esys.finley` module, see Chapter 8.

The following statements define the `Poisson` class object *mypde* with domain *mydomain* and the right hand side f of the PDE to constant 1:

```
from esys.escript.linearPDEs import Poisson
mypde = Poisson(mydomain)
mypde.setValue(f=1)
```

We have not specified any boundary condition but the `Poisson` class implicitly assumes homogeneous Neuman boundary conditions defined by Equation (2.11). With this boundary condition the BVP we have defined has no unique solution. In fact, with any solution u and any constant C the function $u + C$ becomes a solution as well. We have to add a Dirichlet boundary condition . This is done by defining a characteristic function which has positive values at locations $x = (x_0, x_1)$ where Dirichlet boundary condition is set and 0 elsewhere. In our case of Γ^D defined by Equation (2.13), we need to construct a function *gammaD* which is positive for the cases $x_0 = 0$ or $x_1 = 0$. To get an object *x* which contains the coordinates of the nodes in the domain use

```
x=mydomain.getX()
```

The method `getX` of the `Domain` *mydomain* gives access to locations in the domain defined by *mydomain*. The object *x* is actually a `Data` object which will be discussed in Chapter 3 in more detail. What we need to know here is that

x has rank (number of dimensions) and a shape (list of dimensions) which can be viewed by calling the `getRank` and `getShape` methods:

```
print "rank ",x.getRank(),", shape ",x.getShape()
```

This will print something like

```
rank 1, shape (2,)
```

The `Data` object also maintains type information which is represented by the `FunctionSpace` of the object. For instance

```
print x.getFunctionSpace()
```

will print

```
Function space type: Finley_Nodes on FinleyMesh
```

which tells us that the coordinates are stored on the nodes of (rather than on points in the interior of) a `esys.finley` mesh. To get the x_0 coordinates of the locations we use the statement

```
x0=x[0]
```

Object *x0* is again a `Data` object now with rank 0 and shape $()$. It inherits the `FunctionSpace` from *x*:

```
print x0.getRank(),x0.getShape(),x0.getFunctionSpace()
```

will print

```
0 () Function space type: Finley_Nodes on FinleyMesh
```

We can now construct a function *gammaD* which is only non-zero on the bottom and left edges of the domain with

```
from esys.escript import whereZero
gammaD=whereZero(x[0])+whereZero(x[1])
```

`whereZero(x[0])` creates function which equals 1 where `x[0]` is (almost) equal to zero and 0 elsewhere. Similarly, `whereZero(x[1])` creates function which equals 1 where `x[1]` is equal to zero and 0 elsewhere. The sum of the results of `whereZero(x[0])` and `whereZero(x[1])` gives a function on the domain *mydomain* which is strictly positive where x_0 or x_1 is equal to zero. Note that *gammaD* has the same rank , shape and `FunctionSpace` like *x0* used to define it. So from

```
print gammaD.getRank(),gammaD.getShape(),gammaD.getFunctionSpace()
```

one gets

```
0 () Function space type: Finley_Nodes on FinleyMesh
```

An additional parameter *q* of the `setValue` method of the `Poisson` class defines the characteristic function of the locations of the domain where homogeneous Dirichlet boundary condition are set. The complete definition of our example is now:

```
from esys.linearPDEs import Poisson
x = mydomain.getX()
gammaD = whereZero(x[0])+whereZero(x[1])
mypde = Poisson(domain=mydomain)
mypde.setValue(f=1,q=gammaD)
```

The first statement imports the `Poisson` class definition from the `esys.escript.linearPDEs` module `esys.escript` package. To get the solution of the Poisson equation defined by *mypde* we just have to call its `getSolution`.

Now we can write the script to solve our Poisson problem

```
from esys.escript import *
from esys.escript.linearPDEs import Poisson
from esys.finley import Rectangle
# generate domain:
mydomain = Rectangle(l0=1.,l1=1.,n0=40, n1=20)
# define characteristic function of Gamma^D
x = mydomain.getX()
gammaD = whereZero(x[0])+whereZero(x[1])
# define PDE and get its solution u
mypde = Poisson(domain=mydomain)
mypde.setValue(f=1,q=gammaD)
u = mypde.getSolution()
# write u to an external file
saveVTK("u.xml",sol=u)
```

The entire code is available as 'poisson.py' in the example directory

The last statement writes the solution (tagged with the name "sol") to a file named 'u.xml' in *VTK* file format. Now you may run the script and visualize the solution using *mayavi*:

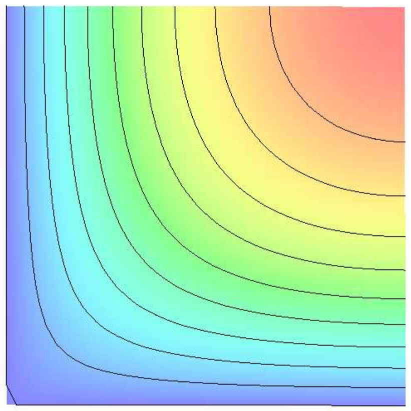


FIGURE 2.3: Visualization of the Poisson Equation Solution for $f = 1$

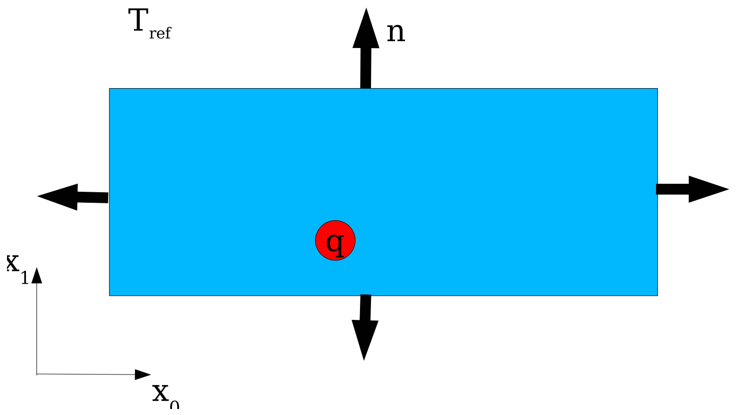


FIGURE 2.4: Temperature Diffusion Problem with Circular Heat Source

```
python poisson.py
mayavi -d u.xml -m SurfaceMap
```

See Figure 2.3.

2.2 The Diffusion Problem

2.2.1 Outline

In this chapter we will discuss how to solve a time-dependent temperature diffusion PDE for a given block of material. Within the block there is a heat source which drives the temperature diffusion. On the surface, energy can radiate into the surrounding environment. Figure 2.4 shows the configuration.

In the next Section 2.2.2 we will present the relevant model. A time integration scheme is introduced to calculate the temperature at given time nodes $t^{(n)}$. We will see that at each time step a Helmholtz equation must be solved. The implementation of a Helmholtz equation solver will be discussed in Section 2.2.3. In Section 2.2.4 the solver of the Helmholtz equation is used to build a solver for the temperature diffusion problem.

2.2.2 Temperature Diffusion

The unknown temperature T is a function of its location in the domain and time $t > 0$. The governing equation in the interior of the domain is given by

$$\rho c_p T_{,t} - (\kappa T_{,i})_{,i} = q_H \tag{2.15}$$

where ρc_p and κ are given material constants. In case of a composite material the parameters depend on their location in the domain. q_H is a heat source (or sink) within the domain. We are using the Einstein summation convention as introduced in Chapter 2.1. In our case we assume q_H to be equal to a constant heat production rate q^c on a circle or sphere with center x^c and radius r and 0 elsewhere:

$$q_H(x,t) = \begin{cases} q^c & \|x - x^c\| \le r \\ & \text{if} \\ 0 & \text{else} \end{cases} \tag{2.16}$$

for all x in the domain and all time $t > 0$.

On the surface of the domain we are specifying a radiation condition which prescribes the normal component of the flux $\kappa T_{,i}$ to be proportional to the difference of the current temperature to the surrounding temperature T_{ref}:

$$\kappa T_{,i} n_i = \eta (T_{ref} - T) \tag{2.17}$$

η is a given material coefficient depending on the material of the block and the surrounding medium. n_i is the i-th component of the outer normal field at the surface of the domain.

To solve the time-dependent Equation (2.15) the initial temperature at time $t = 0$ has to be given. Here we assume that the initial temperature is the surrounding temperature:

$$T(x, 0) = T_{ref} \tag{2.18}$$

for all x in the domain. It is pointed out that the initial conditions satisfy the boundary condition defined by Equation (2.17).

The temperature is calculated at discrete time nodes $t^{(n)}$ where $t^{(0)} = 0$ and $t^{(n)} = t^{(n-1)} + h$ where $h > 0$ is the step size which is assumed to be constant. In the following the upper index (n) refers to a value at time $t^{(n)}$. The simplest and most robust scheme to approximate the time derivative of the the temperature is the backward Euler scheme. The backward Euler scheme is based on the Taylor expansion of T at time $t^{(n)}$:

$$T^{(n)} \approx T^{(n-1)} + T^{(n)}_{,t} (t^{(n)} - t^{(n-1)}) = T^{(n-1)} + h \cdot T^{(n)}_{,t} \tag{2.19}$$

This is inserted into Equation (2.15). By separating the terms at $t^{(n)}$ and $t^{(n-1)}$ one gets for $n = 1, 2, 3 \ldots$

$$\frac{\rho c_p}{h} T^{(n)} - (\kappa T^{(n)}_{,i})_{,i} = q_H + \frac{\rho c_p}{h} T^{(n-1)} \tag{2.20}$$

where $T^{(0)} = T_{ref}$ is taken form the initial condition given by Equation (2.18). Together with the natural boundary condition

$$\kappa T^{(n)}_{,i} n_i = \eta (T_{ref} - T^{(n)}) \tag{2.21}$$

taken from Equation (2.17) this forms a boundary value problem that has to be solved for each time step. As a first step to implement a solver for the temperature diffusion problem we will first implement a solver for the boundary value problem that has to be solved at each time step.

2.2.3 Helmholtz Problem

The partial differential equation to be solved for $T^{(n)}$ has the form

$$\omega T^{(n)} - (\kappa T^{(n)}_{,i})_{,i} = f \tag{2.22}$$

and we set

$$\omega = \frac{\rho c_p}{h} \text{ and } f = q_H + \frac{\rho c_p}{h} T^{(n-1)} \ . \tag{2.23}$$

With $g = \eta T_{ref}$ the radiation condition defined by Equation (2.21) takes the form

$$\kappa T^{(n)}_{,i} n_i = g - \eta T^{(n)} \text{ on } \Gamma \tag{2.24}$$

The partial differential Equation (2.22) together with boundary conditions of Equation (2.24) is called the Helmholtz equation .

We want to use the `LinearPDE` class provided by `esys.escript` to define and solve a general linear,steady, second order PDE such as the Helmholtz equation. For a single PDE the `LinearPDE` class supports the following form:

$$-(A_{jl} u_{,l})_{,j} + Du = Y \ . \tag{2.25}$$

where we show only the coefficients relevant for the problem discussed here. For the general form of single PDE see Equation (4.1). The coefficients A, and Y have to be specified through `Data` objects in the general `FunctionSpace` on the PDE or objects that can be converted into such `Data` objects. A is a rank-2 `Data` object and D and Y are scalar. The following natural boundary conditions are considered on Γ:

$$n_j A_{jl} u_{,l} + du = y \ . \tag{2.26}$$

Notice that the coefficient A is the same like in the PDE Equation (2.25). The coefficients d and y are each a scalar `Data` object in the boundary `FunctionSpace`. Constraints for the solution prescribing the value of the solution at certain locations in the domain. They have the form

$$u = r \text{ where } q > 0 \tag{2.27}$$

r and q are each scalar `Data` object where q is the characteristic function defining where the constraint is applied. The constraints defined by Equation (2.27) override any other condition set by Equation (2.25) or Equation (2.26). The `Poisson` class of the `esys.escript.linearPDEs` module, which we have already used in Chapter 2.1, is in fact a subclass of the more general `LinearPDE` class. The `esys.escript.linearPDEs` module provides a `Helmholtz` class but we will make direct use of the general `LinearPDE` class.

By inspecting the Helmholtz equation (2.22) and boundary condition (2.24) and substituting u for $T^{(n)}$ we can easily assign values to the coefficients in the general PDE of the `LinearPDE` class:

$$\begin{array}{lll} A_{ij} = \kappa \delta_{ij} & D = \omega & Y = f \\ d = \eta & y = g & \end{array} \tag{2.28}$$

δ_{ij} is the Kronecker symbol defined by $\delta_{ij} = 1$ for $i = j$ and 0 otherwise. Undefined coefficients are assumed to be not present.[3] In this diffusion example we do not need to define a characteristic function q because the boundary conditions we consider in Equation (2.24) are just the natural boundary conditions which are already defined in the `LinearPDE` class (shown in Equation (2.26)).

The Helmholtz equation can be set up by following way [4] :

```
mypde=LinearPDE(mydomain)
mypde.setValue(A=kappa*kronecker(mydomain),D=omega,Y=f,d=eta,y=g)
u=mypde.getSolution()
```

where we assume that `mydomain` is a `Domain` object and `kappa` `omega` `eta` and `g` are given scalar values typically `float` or `Data` objects. The `setValue` method assigns values to the coefficients of the general PDE. The `getSolution` method solves the PDE and returns the solution `u` of the PDE. `kronecker` is `esys.escript` function returning the Kronecker symbol.

The coefficients can set by several calls of `setValue` where the order can be chosen arbitrarily. If a value is assigned to a coefficient several times, the last assigned value is used when the solution is calculated:

```
mypde=LinearPDE(mydomain)
mypde.setValue(A=kappa*kronecker(mydomain),d=eta)
mypde.setValue(D=omega,Y=f,y=g)
mypde.setValue(d=2*eta) # overwrites d=eta
u=mypde.getSolution()
```

[3] There is a difference in `esys.escript` of being not present and set to zero. As not present coefficients are not processed, it is more efficient to leave a coefficient undefined instead of assigning zero to it.

[4] Please, note that this is not a complete code. The complete code can be found in "helmholtz.py".

In some cases the solver of the PDE can make use of the fact that the PDE is symmetric where the PDE is called symmetric if

$$A_{jl} = A_{lj} \ . \tag{2.29}$$

Note that D and d may have any value and the right hand sides Y, y as well as the constraints are not relevant. The Helmholtz problem is symmetric. The `LinearPDE` class provides the method `checkSymmetry` method to check if the given PDE is symmetric.

```
mypde=LinearPDE(mydomain)
mypde.setValue(A=kappa*kronecker(mydomain),d=eta)
print mypde.checkSymmetry() # returns True
mypde.setValue(B=kronecker(mydomain)[0])
print mypde.checkSymmetry() # returns False
mypde.setValue(C=kronecker(mydomain)[0])
print mypde.checkSymmetry() # returns True
```

Unfortunately, a `checkSymmetry` is very expensive and is recommendable to use for testing and debugging purposes only. The `setSymmetryOn` method is used to declare a PDE symmetric:

```
mypde = LinearPDE(mydomain)
mypde.setValue(A=kappa*kronecker(mydomain))
mypde.setSymmetryOn()
```

Now we want to see how we actually solve the Helmholtz equation. on a rectangular domain of length $l_0 = 5$ and height $l_1 = 1$. We choose a simple test solution such that we can verify the returned solution against the exact answer. Actually, we take $T = x_0$ (here $q_H = 0$) and then calculate the right hand side terms f and g such that the test solution becomes the solution of the problem. If we assume κ as being constant, an easy calculation shows that we have to choose $f = \omega \cdot x_0$. On the boundary we get $\kappa n_i u_{,i} = \kappa n_0$. So we have to set $g = \kappa n_0 + \eta x_0$. The following script 'helmholtz.py' which is available in the example directory implements this test problem using the `esys.finley` PDE solver:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Rectangle
#... set some parameters ...
kappa=1.
omega=0.1
eta=10.
#... generate domain ...
mydomain = Rectangle(l0=5.,l1=1.,n0=50, n1=10)
#... open PDE and set coefficients ...
mypde=LinearPDE(mydomain)
mypde.setSymmetryOn()
n=mydomain.getNormal()
x=mydomain.getX()
mypde.setValue(A=kappa*kronecker(mydomain),D=omega,Y=omega*x[0], \
               d=eta,y=kappa*n[0]+eta*x[0])
#... calculate error of the PDE solution ...
u=mypde.getSolution()
print "error is ",Lsup(u-x[0])
saveVTK("x0.xml",sol=u)
```

To visualize the solution 'x0. xml' just use the command

```
mayavi -d u.xml -m SurfaceMap &
```

and it is easy to see that the solution $T = x_0$ is calculated.

The script is similar to the script 'poisson.py' discussed in Chapter 2.1. `mydomain.getNormal()` returns the outer normal field on the surface of the domain. The function `Lsup` imported by the `from esys.escript import *` statement and returns the maximum absolute value of its argument. The error shown by the print statement should be in the order of 10^{-7}. As piecewise bi-linear interpolation is used by `esys.finley` approximate the solution and our solution is a linear function of the spatial coordinates one might expect that the error would be zero or in the order of machine precision (typically $\approx 10^{-15}$). However most PDE packages use an iterative solver which is terminated when a given tolerance has been reached. The default tolerance is 10^{-8}. This value can be altered by using the `setTolerance` of the `LinearPDE` class.

2.2.4 The Transition Problem

Now we are ready to solve the original time-dependent problem. The main part of the script is the loop over time t which takes the following form:

```
t=0
T=Tref
mypde=LinearPDE(mydomain)
mypde.setValue(A=kappa*kronecker(mydomain),D=rhocp/h,d=eta,y=eta*Tref)
while t<t_end:
      mypde.setValue(Y=q+rhocp/h*T)
      T=mypde.getSolution()
      t+=h
```

kappa, *rhocp*, *eta* and *Tref* are input parameters of the model. *q* is the heat source in the domain and *h* is the time step size. The variable *T* holds the current temperature. It is used to calculate the right hand side coefficient *f* in the Helmholtz equation in Equation (2.22). The statement `T=mypde.getSolution()` overwrites *T* with the temperature of the new time step $t+h$. To get this iterative process going we need to specify the initial temperature distribution, which equal to T_{ref}. The `LinearPDE` class object *mypde* and coefficients not changing over time are set up before the loop over time is entered. In each time step only the coefficient Y is reset as it depends on the temperature of the previous time step. This allows the PDE solver to reuse information from previous time steps as much as possible.

The heat source q_H which is defined in Equation (2.16) is *qc* in an area defined as a circle of radius *r* and center *xc* and zero outside this circle. *q0* is a fixed constant. The following script defines q_H as desired:

```
from esys.escript import length,whereNegative
xc=[0.02,0.002]
r=0.001
x=mydomain.getX()
qH=q0*whereNegative(length(x-xc)-r)
```

x is a `Data` class object of the `esys.escript` module defining locations in the `Domain` *mydomain*. The `length()` imported from the `esys.escript` module returns the Euclidean norm:

$$\|y\| = \sqrt{y_i y_i} = \texttt{esys.escript.length}(y) \tag{2.30}$$

So `length(x-xc)` calculates the distances of the location *x* to the center of the circle *xc* where the heat source is acting. Note that the coordinates of *xc* are defined as a list of floating point numbers. It is automatically converted into a `Data` class object before being subtracted from *x*. The function `whereNegative` applied to `length(x-xc)-r`, returns a `Data` object which is equal to one where the object is negative (inside the circle) and zero elsewhere. After multiplication with *qc* we get a function with the desired property of having value *qc* inside the circle and zero elsewhere.

Now we can put the components together to create the script 'diffusion.py' which is available in the example directory: :

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Rectangle
#... set some parameters ...
xc=[0.02,0.002]
r=0.001
qc=50.e6
Tref=0.
rhocp=2.6e6
eta=75.
kappa=240.
tend=5.
# ... time, time step size and counter ...
```

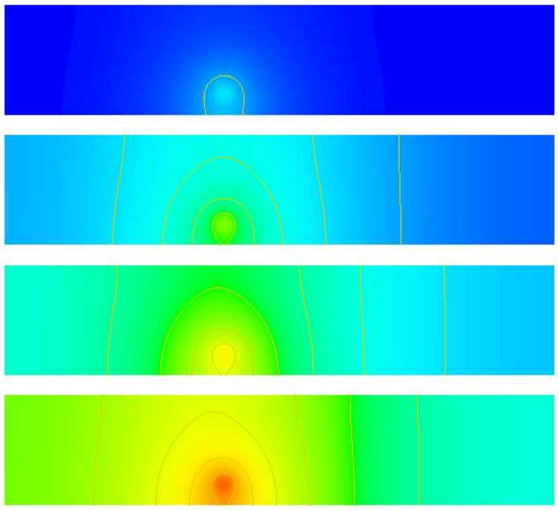


FIGURE 2.5: Results of the Temperature Diffusion Problem for Time Steps 1 16, 32 and 48.

```
t=0
h=0.1
i=0
#... generate domain ...
mydomain = Rectangle(l0=0.05,l1=0.01,n0=250, n1=50)
#... open PDE ...
mypde=LinearPDE(mydomain)
mypde.setSymmetryOn()
mypde.setValue(A=kappa*kronecker(mydomain),D=rhocp/h,d=eta,y=eta*Tref)
# ... set heat source: ....
x=mydomain.getX()
qH=qc*whereNegative(length(x-xc)-r)
# ... set initial temperature ....
T=Tref
# ... start iteration:
while t<tend:
      i+=1
      t+=h
      print "time step :",t
      mypde.setValue(Y=qH+rhocp/h*T)
      T=mypde.getSolution()
      saveVTK("T.%d.xml"%i,temp=T)
```

The script will create the files 'T.1.xml', 'T.2.xml', . . ., 'T.50.xml' in the directory where the script has been started. The files give the temperature distributions at time steps $1, 2, \ldots, 50$ in the *VTK* file format.

Figure 2.5 shows the result for some selected time steps. An easy way to visualize the results is the command

```
mayavi -d T.1.xml -m SurfaceMap &
```

Use the `Configure Data` window in mayavi to move forward and and backwards in time.

2.3 3-D Wave Propagation

In this next example we want to calculate the displacement field u_i for any time $t > 0$ by solving the wave equation:

$$\rho u_{i,tt} - \sigma_{ij,j} = 0 \tag{2.31}$$

in a three dimensional block of length L in x_0 and x_1 direction and height H in x_2 direction. ρ is the known density which may be a function of its location. σ_{ij} is the stress field which in case of an isotropic, linear elastic material is given by

$$\sigma_{ij} \quad = \quad \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i}) \tag{2.32}$$

where λ and μ are the Lame coefficients and δ_{ij} denotes the Kronecker symbol. On the boundary the normal stress is given by

$$\sigma_{ij}n_j = 0 \tag{2.33}$$

for all time $t > 0$.

At initial time $t = 0$ the displacement u_i and the velocity $u_{i,t}$ are given:

$$u_i(0,x) = \begin{cases} U_0 & \text{for } x \text{ at point charge, } x_C \\ 0 & \text{elsewhere} \end{cases} \quad \text{and} \quad u_{i,t}(0,x) = 0 \tag{2.34}$$

for all x in the domain.

Here we are modelling a point source at the point x_C, in the numerical solution we set the initial displacement to be U_0 in a sphere of small radius around the point x_C.

We use an explicit time integration scheme to calculate the displacement field u at certain time marks $t^{(n)}$ where $t^{(n)} = t^{(n-1)} + h$ with time step size $h > 0$. In the following the upper index (n) refers to values at time $t^{(n)}$. We use the Verlet scheme with constant time step size h which is defined by

$$u^{(n)} = 2u^{(n-1)} - u^{(n-2)} + h^2 a^{(n)} \tag{2.35}$$

(2.36)

for all $n = 2, 3, \ldots$. It is designed to solve a system of equations of the form

$$u_{,tt} = G(u) \tag{2.37}$$

where one sets $a^{(n)} = G(u^{(n-1)})$.

In our case $a^{(n)}$ is given by

$$\rho a_i^{(n)} = \sigma_{ij,j}^{(n-1)} \tag{2.38}$$

and boundary conditions

$$\sigma_{ij}^{(n-1)} n_j = 0 \tag{2.39}$$

derived from Equation (2.33) where

$$\sigma_{ij}^{(n-1)} \quad = \quad \lambda u_{k,k}^{(n-1)}\delta_{ij} + \mu(u_{i,j}^{(n-1)} + u_{j,i}^{(n-1)}). \tag{2.40}$$

Now we have converted our problem for displacement, $u^{(n)}$, into a problem for acceleration, $a^(n)$, which now depends on the solution at the previous two time steps, $u^{(n-1)}$ and $u^{(n-2)}$.

In each time step we have to solve this problem to get the acceleration $a^{(n)}$, and we will use the `LinearPDE` class of the `esys.escript.linearPDEs` to do so. The general form of the PDE defined through the `LinearPDE` class is discussed in Section 4.1. The form which is relevant here is

$$D_{ij}a_j^{(n)} = -X_{ij,j} \ . \tag{2.41}$$

The natural boundary condition

$$n_j X_{ij} = 0 \tag{2.42}$$

is used.

With $u = a^{(n)}$ we can identify the values to be assigned to D and X:

$$D_{ij} = \rho\delta_{ij} \quad X_{ij} = -\sigma_{ij}^{(n-1)} \tag{2.43}$$

The following script defines a the function `wavePropagation` which implements the Verlet scheme to solve our wave propagation problem. The argument *domain* which is a `Domain` class object defines the domain of the problem. *h* and *tend* are the time step size and the end time of the simulation. *lam*, *mu* and *rho* are material properties.

```
from esys.linearPDEs import LinearPDE
from numarray import identity,zeros,ones
from esys.escript import *
from esys.escript.pdetools import Locator
def wavePropagation(domain,h,tend,lam,mu,rho,U0):
   x=domain.getX()
   # ... open new PDE ...
   mypde=LinearPDE(domain)
   mypde.setSolverMethod(LinearPDE.LUMPING)
   kronecker=identity(mypde.getDim())
   #  spherical source at middle of bottom face
   xc=[width/2.,width/2.,0.]
   # define small radius around point xc
   # Lsup(x) returns the maximum value of the argument x
   src_radius = 0.1*Lsup(domain.getSize())
   print "src_radius = ",src_radius
   dunit=numarray.array([1.,0.,0.]) # defines direction of point source
   mypde.setValue(D=kronecker*rho)
   # ... set initial values ....
   n=0
   # initial value of displacement at point source is constant (U0=0.01)
   # for first two time steps
   u=U0*whereNegative(length(x-xc)-src_radius)*dunit
   u_last=U0*whereNegative(length(x-xc)-src_radius)*dunit
   t=0
   # define the location of the point source
   L=Locator(domain,xc)
   # find potential at point source
   u_pc=L.getValue(u)
   print "u at point charge=",u_pc
   u_pc_x = u_pc[0]
   u_pc_y = u_pc[1]
   u_pc_z = u_pc[2]
   # open file to save displacement at point source
   u_pc_data=open('./data/U_pc.out','w')
   u_pc_data.write("%f %f %f %f\n"%(t,u_pc_x,u_pc_y,u_pc_z))
   while t<tend:
     # ... get current stress ....
     g=grad(u)
     stress=lam*trace(g)*kronecker+mu*(g+transpose(g))
     # ... get new acceleration ....
     mypde.setValue(X=-stress)
     a=mypde.getSolution()
     # ... get new displacement ...
     u_new=2*u-u_last+h**2*a
     # ... shift displacements ....
     u_last=u
     u=u_new
     t+=h
     n+=1
     print n,"-th time step t ",t
     L=Locator(domain,xc)
     u_pc=L.getValue(u)
     print "u at point charge=",u_pc
     u_pc_x=u_pc[0]
     u_pc_y=u_pc[1]
     u_pc_z=u_pc[2]
     # save displacements at point source to file for t > 0
     u_pc_data.write("%f %f %f %f\n"%(t,u_pc_x,u_pc_y,u_pc_z))
     # ... save current acceleration in units of gravity and displacements
     if n==1 or n%10==0: saveVTK("./data/usoln.%i.vtu"%(n/10),acceleration=length(a)/9.81,
     displacement = length(u), Ux = u[0] )
   u_pc_data.close()
```

Notice that all coefficients of the PDE which are independent of time t are set outside the `while` loop. This is very efficient since it allows the `LinearPDE` class to reuse information as much as possible when iterating over time.

there are a few new `esys.escript` functions in this example: `grad(u)` returns the gradient $u_{i,j}$ of u (in fact *grad(g)[i,j]==* $u_{i,j}$). There are restrictions on the argument of the `grad` function, for instance the statement `grad(grad(u))` will raise an exception. `trace(g)` returns the sum of the main diagonal elements *g[k,k]* of *g* and `transpose(g)` returns the matrix transpose of *g* (ie. *transpose(g)[i,j]* $=$ *g[j,i]*).

We initialize the values of `u` and `u_last` to be U_0 for a small sphere of radius, `src_radius` around the point source located at x_C. These satisfy the initial conditions defined in Equation (2.34).

The output `U_pc.out` and `vtu` files are saved in a directory called `data`. The `U_pc.out` stores 4 columns of data: t, u_x, u_y, u_z respectively, where u_x, u_y, u_z are the x_0, x_1, x_2 components of the displacement vector u at the point source. These can be plotted easily using any plotting package. In gnuplot the command: `plot 'U_pc.out' u 1:2 title 'U_x' w l lw 2, 'U_pc.out' u 1:3 title 'U_y' w l lw 2, 'U_pc.out' u 1:4 title 'U_z' w l lw 2` will reproduce Figure 2.6.

The statement `myPDE.setLumpingOn()` switches on the use of an aggressive approximation of the PDE operator as a diagonal matrix formed from the coefficient *D*. The approximation allows, at the cost of additional error, very fast solution of the PDE. When using `setLumpingOn` the presence of *A*, *B* or *C* will produce wrong results.

One of the big advantages of the Verlet scheme is the fact that the problem to be solved in each time step is very simple and does not involve any spatial derivatives (which is what allows us to use lumping in this simulation). The problem becomes so simple because we use the stress from the last time step rather then the stress which is actually present at the current time step. Schemes using this approach are called an explicit time integration schemes . The backward Euler scheme we have used in Chapter 2.2 is an example of an implicit scheme . In this case one uses the actual status of each variable at a particular time rather then values from previous time steps. This will lead to a problem which is more expensive to solve, in particular for non-linear problems. Although explicit time integration schemes are cheap to finalize a single time step, they need significantly smaller time steps then implicit schemes and can suffer from stability problems. Therefore they need a very careful selection of the time step size h.

An easy, heuristic way of choosing an appropriate time step size is the Courant condition which says that within a time step a information should not travel further than a cell used in the discretization scheme. In the case of the wave equation the velocity of a (p-) wave is given as $\sqrt{\frac{\lambda+2\mu}{\rho}}$ so one should choose h from

$$h = \frac{1}{5}\sqrt{\frac{\rho}{\lambda+2\mu}}\Delta x \tag{2.44}$$

where Δx is the cell diameter. The factor $\frac{1}{5}$ is a safety factor considering the heuristics of the formula.

The following script uses the `wavePropagation` function to solve the wave equation for a point source located at the bottom face of a block. The width of the block in each direction on the bottom face is 10km (x_0 and x_1 directions ie. `l0` and `l1`). The `ne` gives the number of elements in x_0 and x_1 directions. The depth of the block is aligned with the x_2-direction. The depth (`l2`) of the block in the x_2-direction is chosen so that there are 10 elements and the magnitude of the of the depth is chosen such that the elements become cubic. We chose 10 for the number of elements in x_2-direction so that the computation would be faster. `Brick(`$n_0, n_1, n_2, l_0, l_1, l_2$`)` is an `esys.finley` function which creates a rectangular mesh with $n_0 \times n_1 \times n_2$ elements over the brick $[0, l_0] \times [0, l_1] \times [0, l_2]$.

```
from esys.finley import Brick
ne=32          # number of cells in x_0 and x_1 directions
width=10000.  # length in x_0 and x_1 directions
lam=3.462e9
mu=3.462e9
rho=1154.
tend=60
h=(1./5.)*sqrt(rho/(lam+2*mu))*(width/ne)
print "time step size = ",h
U0=0.01 # amplitude of point source
```

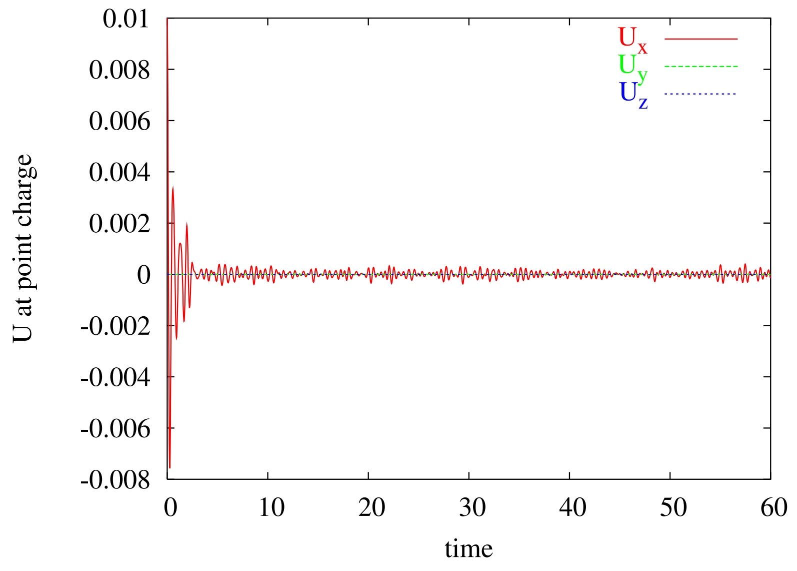


FIGURE 2.6: Amplitude at Point source

```
mydomain=Brick(ne,ne,10,l0=width,l1=width,l2=10.*width/32.)
wavePropagation(mydomain,h,tend,lam,mu,rho,U0)
```

The script is available as 'wave.py' in the example directory . Before running the code make sure you have created a directory called `data` in the current working directory. To visualize the results from the data directory:

```
mayavi -d usoln.1.vtu -m SurfaceMap &
```

You can rotate this figure by clicking on it with the mouse and moving it around. Again use `Configure Data` to move backwards and forward in time, and also to choose the results (acceleration, displacement or u_x) by using `Select Scalar`. Figure 2.7 shows the results for the displacement at various time steps.

2.4 Elastic Deformation

In this section we want to examine the deformation of a linear elastic body caused by expansion through a heat distribution. We want a displacement field u_i which solves the momentum equation :

$$-\sigma_{ij,j} = 0 \tag{2.45}$$

where the stress σ is given by

$$\sigma_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i}) - (\lambda + \frac{2}{3}\mu)\ \alpha\ (T - T_{ref})\delta_{ij}\ . \tag{2.46}$$

In this formula λ and μ are the Lame coefficients, α is the temperature expansion coefficient, T is the temperature distribution and $Tref$ a reference temperature. Note that Equation (2.45) is similar to eqnWAVE general problem introduced in section Section 2.3 but the inertia term $\rho u_{i,tt}$ has been dropped as we assume a static scenario here. Moreover, in comparison to the Equation (2.32) definition of stress σ in Equation (2.46) an extra term is introduced to bring in stress due to volume changes trough temperature dependent expansion.

Our domain is the unit cube

$$\Omega = \{(x_i | 0 \leq x_i \leq 1\} \tag{2.47}$$

On the boundary the normal stress component is set to zero

$$\sigma_{ij}n_j = 0 \tag{2.48}$$

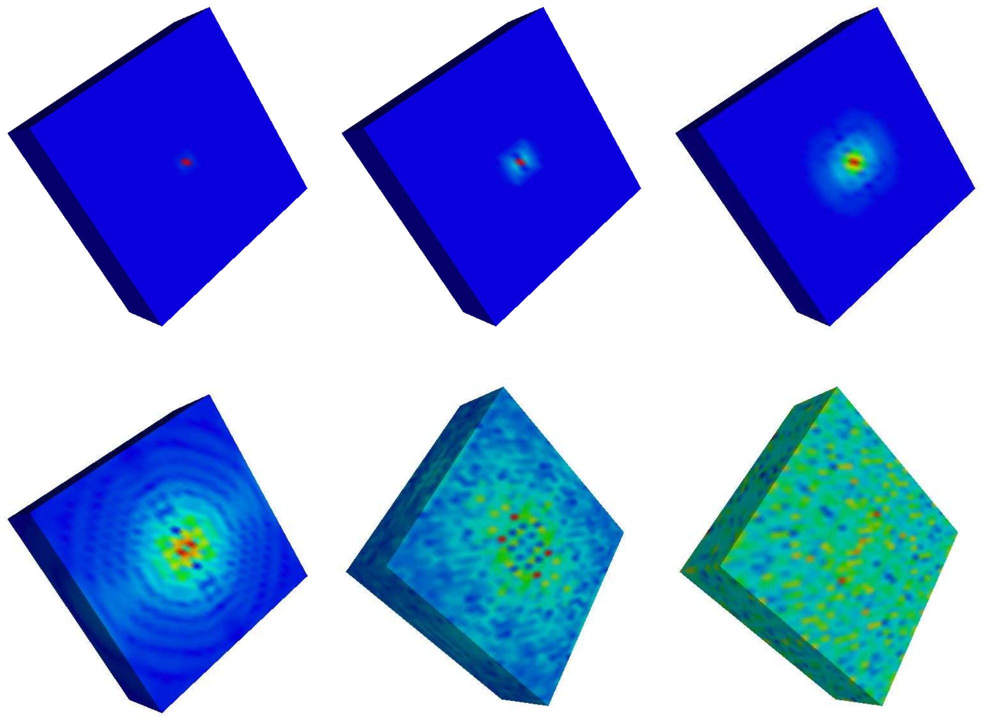


FIGURE 2.7: Selected time steps ($n = 0, 1, 30, 100, 300$ and 2880) of a wave propagation over a 10km $\times$ 10km $\times$ 3.125km block from a point source initially at $(5\text{km}, 5\text{km}, 0)$ with time step size $h = 0.02083$. Color represents the displacement. Here the view is oriented onto the bottom face.

and on the face with $x_i = 0$ we set the i-th component of the displacement to 0

$$u_i(x) = 0 \quad \text{where} \quad x_i = 0 \tag{2.49}$$

For the temperature distribution we use

$$T(x) = T_0 e^{-\beta \|x - x^c\|}; \tag{2.50}$$

with a given positive constant β and location x^c in the domain. Later in Section **??** we will use T from a time-dependent temperature diffusion problem as discussed in Section 2.2.

When we insert Equation (2.46) we get a second order system of linear PDEs for the displacements u which is called the Lame equation. We want to solve this using the `LinearPDE` class to this. For a system of PDEs and a solution with several components the `LinearPDE` class takes PDEs of the form

$$-A_{ijkl} u_{k,l}), j = -X_{ij,j} \; . \tag{2.51}$$

A is of rank-4 `Data` object and X is of rank-2 `Data` object. We show here the coefficients relevant for the we trying to solve. The full form is given in Equation (4.4). The natural boundary conditions take the form:

$$n_j A_{ijkl} u_{k,l} = n_j X_{ij} \; . \tag{2.52}$$

Constraints take the form

$$u_i = r_i \text{ where } q_i > 0 \tag{2.53}$$

r and q are each rank-1 `Data` object. We can easily identify the coefficients in Equation (2.51):

$$A_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{2.54}$$

$$X_{ij} = (\lambda + \frac{2}{3}\mu) \; \alpha \; (T - T_{ref})\delta_{ij} \tag{2.55}$$

$$\tag{2.56}$$

The characteristic function q defining the locations and components where constraints are set is given by:

$$q_i(x) = \begin{cases} 1 & x_i = 0 \\ 0 & \text{otherwise} \end{cases} \tag{2.57}$$

Under the assumption that λ, μ, β and T_{ref} are constant we may use $Y_i = \lambda + \frac{2}{3}\mu)\ \alpha\ T_i$. However, this choice would lead to a different natural boundary condition which does not set the normal stress component as defined in Equation (2.46) to zero.

Analogously to concept of symmetry for a single PDE, we call the PDE defined by Equation (2.51) symmetric if

$$A_{ijkl} = A_{klij} \tag{2.58}$$

$$\tag{2.59}$$

This Lame equation is in fact symmetric, given the difference in D and d as compared to the scalar case. The `LinearPDE` class is notified of this fact by calling its `setSymmetryOn` method.

After we have solved the Lame equation we want to analyse the actual stress distribution. Typically the von–Mises stress defined by

$$\sigma_{mises} = \sqrt{\frac{1}{6}((\sigma_{00} - \sigma_{11})^2 + (\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{00})^2) + \sigma_{01}^2 + \sigma_{12}^2 + \sigma_{20}^2} \tag{2.60}$$

is used to detect material damage. Here we want to calculate the von–Mises and write the stress to a file for visualization.

The following script, which is available in ‘heatedbox.py’ in the example directory, solves the Lame equation and writes the displacements and the von–Mises stress into a file ‘deform.xml’ in the *VTK* file format:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Brick
#... set some parameters ...
lam=1.
mu=0.1
alpha=1.e-6
xc=[0.3,0.3,1.]
beta=8.
T_ref=0.
T_0=1.
#... generate domain ...
mydomain = Brick(l0=1.,l1=1., l2=1.,n0=10, n1=10, n2=10)
x=mydomain.getX()
#... set temperature ...
T=T_0*exp(-beta*length(x-xc))
#... open symmetric PDE ...
mypde=LinearPDE(mydomain)
mypde.setSymmetryOn()
#... set coefficients ...
C=Tensor4(0.,Function(mydomain))
for i in range(mydomain.getDim()):
  for j in range(mydomain.getDim()):
     C[i,i,j,j]+=lam
     C[j,i,j,i]+=mu
     C[j,i,i,j]+=mu
msk=whereZero(x[0])*[1.,0.,0.] \
   +whereZero(x[1])*[0.,1.,0.] \
   +whereZero(x[2])*[0.,0.,1.]
sigma0=(lam+2./3.*mu)*alpha*(T-T_ref)*kronecker(mydomain)
mypde.setValue(A=C,X=sigma0,q=msk)
#... solve pde ...
u=mypde.getSolution()
#... calculate von-Misses stress
g=grad(u)
sigma=mu*(g+transpose(g))+lam*trace(g)*kronecker(mydomain)-sigma0
```

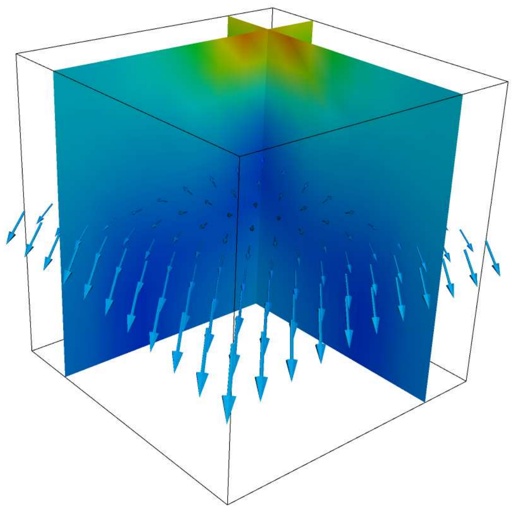


FIGURE 2.8: von–Mises Stress and Displacement Vectors.

```
sigma_mises=sqrt(((sigma[0,0]-sigma[1,1])**2+(sigma[1,1]-sigma[2,2])**2+ \
                  (sigma[2,2]-sigma[0,0])**2)/6. \
                 +sigma[0,1]**2 + sigma[1,2]**2 + sigma[2,0]**2)
#... output ...
saveVTK("deform.xml",disp=u,stress=sigma_mises)
```

Finally the the results can be visualize by calling

```
mayavi -d deform.xml -f CellToPointData -m VelocityVector -m SurfaceMap &
```

Note that the filter CellToPointData is applied to create smooth representation of the von–Mises stress. Figure 2.8 shows the results where the vertical planes showing the von–Mises stress and the horizontal plane shows the vector representing displacements.

2.5 Rayleigh-Taylor Instability

In this chapter we will implement the Level Set Method in Escript for tracking the interface between two fluids for Computational Fluid Dynamics (CFD). The method is tested with a Rayleigh-Taylor Instability problem, which is an instability of the interface between two fluids with differing densities.
Normally in Earth science problems two or more fluids in a system with different properties are of interest. For example, lava dome growth in volcanology, with the contrast of the two mediums as being lava and air. The interface between the two mediums is often referred to as a free surface (free boundary value problem); the problem arises due to the large differences in densities between the lava and air, with their ratio being around 2000, and so the interface between the two fluids move with respect to each other. There are a number of numerical techniques to define and track the free surfaces. One of these methods, which is conceptually the simplest, is to construct a Lagrangian grid which moves with the fluid, and so it tracks the free surface. The limitation of this method is that it cannot track surfaces that break apart or intersect. Another limitation is that the elements in the grid can become severely distorted, resulting in numerical instability. The Arbitrary Lagrangian-Eulerian (ALE) method for CFD in moving domains is used to overcome this problem by remeshing, but there is an overhead in computational time, and it results in a loss of accuracy due to the process of mapping the state variables every remesh by interpolation.

There is a technique to overcome these limitations called the Level Set Method, for tracking interfaces between two fluids. The advantages of the method is that CFD can be performed on a fixed Cartesian mesh, and therefore problems with remeshing can be avoided. The field equations for calculating variables such as velocity and pressure are solved on the the same mesh. The Level Set Method is based upon the implicit representation of

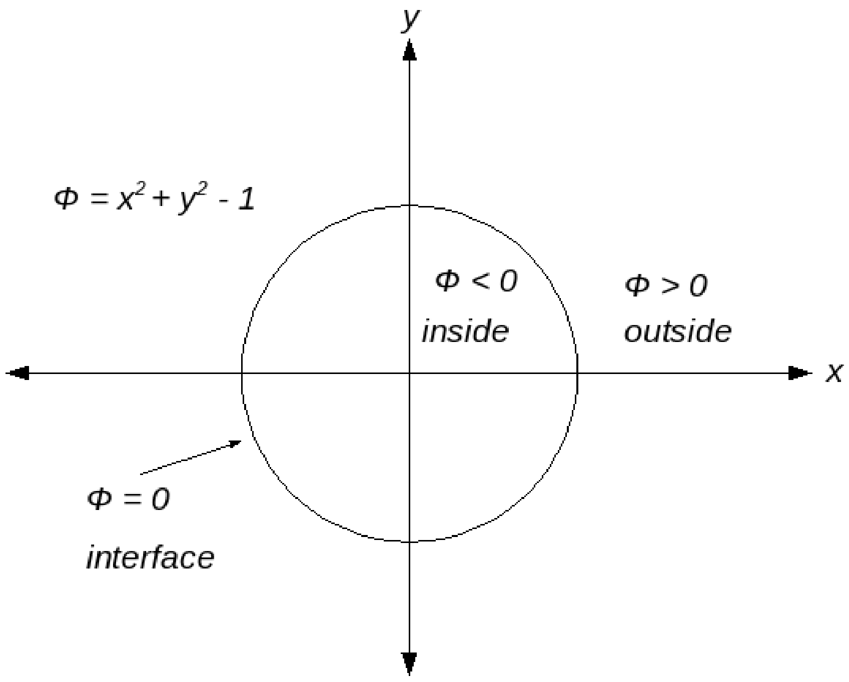


FIGURE 2.9: Implicit representation of the curve $x^2 + y^2 = 1$.

the interface by a continuous function. The function takes the form as a signed distance function, $\phi(x)$, of the interface in a Eulerian coordinate system. For example, the zero isocontour of the unit circle $\phi(x) = x^2 + y^2 - 1$ is the set of all points where $\phi(x) = 0$. Refer to Figure 2.9. The implicit representation can be used to define the interior and exterior of a fluid region. Since the isocontour at $\phi(x) = 0$ has been defined as the interface, a point in the domain can be determined if its inside or outside of the interface, by looking at the local sign of $\phi(x)$. For example, a point is inside the interface when $\phi(x) < 0$, and outside the interface when $\phi(x) > 0$. Parameters values such as density and viscosity can then be defined for two different mediums, depending on which side of the interface they are located.

2.5.1 Calculation of the Displacement of the Interface

The displacement of the interface at the zero isocontour of $\phi(x)$ is calculated each time-step by using the velocity field. This is achieved my solving the advection equation:

$$\frac{\partial \phi}{\partial t} + \vec{v} \cdot \nabla \phi = 0, \tag{2.61}$$

where $\vec{v}$ is the velocity field. The advection equation is solved using a mid-point, which is a two step procedure:

Firstly, $\phi^{1/2}$ is calculated solving:

$$\frac{\phi^{1/2} - \phi^-}{dt/2} + \vec{v} \cdot \nabla \phi^- = 0. \tag{2.62}$$

Secondly, using $\phi^{1/2}$, ϕ^+ is calculated solving:

$$\frac{\phi^+ - \phi^-}{dt} + \vec{v} \cdot \nabla \phi^{1/2} = 0. \tag{2.63}$$

This procedure works provided that the discretization of the left-hand side of Equations (2.62) and (2.63) is a lumped mass matrix. For more details on the mid-point procedure see reference [7]. In certain situations the mid-point procedure has been shown to produce artifacts in the numerical solutions. A more robust procedure is to use the Taylor-Galerkin scheme with the presence of diffusion, which gives more stable solutions. The expression is derived by either inserting Equation (2.62) into Equation (2.63), or by expanding ϕ into a Taylor series:

$$\phi^+ \simeq \phi^- + dt \frac{\partial \phi^-}{\partial t} + \frac{dt^2}{2} \frac{\partial^2 \phi^-}{\partial t^2}, \tag{2.64}$$

by inserting

$$\frac{\partial \phi^-}{\partial t} = -\vec{v} \cdot \nabla \phi^-, \tag{2.65}$$

and

$$\frac{\partial^2 \phi^-}{\partial t^2} = \frac{\partial}{\partial t}(-\vec{v} \cdot \nabla \phi^-) = \vec{v} \cdot \nabla(\vec{v} \cdot \nabla \phi^-), \tag{2.66}$$

into Equation (2.64)

$$\phi^+ = \phi^- - dt\vec{v} \cdot \nabla \phi^- + \frac{dt^2}{2}\vec{v} \cdot \nabla(\vec{v} \cdot \nabla \phi^-). \tag{2.67}$$

2.5.2 Governing Equations for Fluid Flow

The fluid dynamics is governed by the Stokes equations. In geophysical problems the velocity of fluids are low; that is, the inertial forces are small compared with the viscous forces, therefore the inertial terms in the Navier-Stokes equations can be ignored. For a body force f the governing equations are given by:

$$\nabla \cdot (\eta(\nabla \vec{v} + \nabla^T \vec{v})) - \nabla p = -f, \tag{2.68}$$

with the incompressibility condition

$$\nabla \cdot \vec{v} = 0. \tag{2.69}$$

where p, η and f are the pressure, viscosity and body forces, respectively. Alternatively, the Stokes equations can be represented in Einstein summation tensor notation (compact notation):

$$-(\eta(v_{i,j} + v_{j,i})),_j - p,_i = f_i, \tag{2.70}$$

with the incompressibility condition

$$-v_{i,i} = 0. \tag{2.71}$$

The subscript comma i denotes the derivative of the function with respect to x_i. A linear relationship between the deviatoric stress $\sigma^{'}_{ij}$ and the stretching $D_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i})$ is defined as [9]:

$$\sigma^{'}_{ij} = 2\eta D^{'}_{ij}, \tag{2.72}$$

where the deviatoric stretching $D^{'}_{ij}$ is defined as

$$D^{'}_{ij} = D^{'}_{ij} - \frac{1}{3}D_{kk}\delta_{ij}. \tag{2.73}$$

where δ_{ij} is the Kronecker δ-symbol, which is a matrix with ones for its diagonal entries ($i = j$) and zeros for the remaining entries ($i \neq j$). The body force f in Equation (2.70) is the gravity acting in the x_3 direction and is given as $f = -g\rho\delta_{i3}$. The Stokes equations is a saddle point problem, and can be solved using a Uzawa scheme. A class called StokesProblemCartesian in Escript can be used to solve for velocity and pressure. In order to keep numerical stability, the time-step size needs to be below a certain value, known as the Courant number. The Courant number is defined as:

$$C = \frac{v\delta t}{h}. \tag{2.74}$$

where δt, v, and h are the time-step, velocity, and the width of an element in the mesh, respectively. The velocity v may be chosen as the maximum velocity in the domain. In this problem the Courant number is taken to be 0.4 [7].

2.5.3 Reinitialization of Interface

As the computation of the distance function progresses, it becomes distorted, and so it needs to be updated in order to stay regular [15]. This process is known as the reinitialization procedure. The aim is to iteratively find a solution to the reinitialization equation:

$$\frac{\partial \psi}{\partial \tau} + sign(\phi)(1 - \nabla \psi) = 0. \tag{2.75}$$

where ψ shares the same level set with ϕ, τ is pseudo time, and $sign(\phi)$ is the smoothed sign function. This equation is solved to meet the definition of the level set function, $|\nabla\psi| = 1$; the normalization condition. Equation (2.75) can be rewritten in similar form to the advection equation:

$$\frac{\partial\psi}{\partial\tau} + \vec{w}\cdot\nabla\psi = sign(\phi), \tag{2.76}$$

where

$$\vec{w} = sign(\phi)\frac{\nabla\psi}{|\nabla\psi|}. \tag{2.77}$$

$\vec{w}$ is the characteristic velocity pointing outward from the free surface. Equation (2.76) can be solved by a similar technique to what was used in the advection step; either by the mid-point technique [7] or the Taylor-Galerkin procedure. For the mid-point technique, the reinitialization technique algorithm is:

1. Calculate

$$\vec{w} = sign(\phi)\frac{\nabla\psi}{|\nabla\psi|}, \tag{2.78}$$

2. Calculate $\psi^{1/2}$ solving

$$\frac{\psi^{1/2} - \psi^-}{d\tau/2} + \vec{w}\cdot\nabla\psi^- = sign(\phi), \tag{2.79}$$

3. using $\psi^{1/2}$, calculate ψ^+ solving

$$\frac{\psi^+ - \psi^-}{d\tau} + \vec{w}\cdot\nabla\psi^{1/2} = sign(\phi), \tag{2.80}$$

4. if the convergence criterion has not been met, go back to step 2. Convergence is declared if

$$||\nabla\psi_\infty| - 1| < \epsilon_\psi. \tag{2.81}$$

where ϵ is the convergence tolerance. Normally, the reinitialization procedure is performed every third time-step of solving the Stokes equation.

The mid-point technique works provided that the left-hand side of Equations (2.79) and (2.80) is a lumped mass matrix. Alternatively, for a one-step procedure, the reinitialization equation can be given by:

$$\psi^+ = \psi^- - \tau\vec{w}\cdot\nabla\psi^- + \frac{d\tau^2}{2}\vec{w}\cdot\nabla(\vec{w}\cdot\nabla\psi^-). \tag{2.82}$$

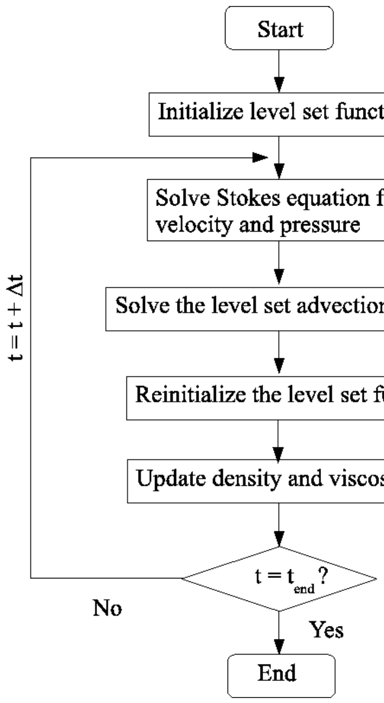
The accuracy of ϕ is only needed within the transition zone; and so it can be calculated in a narrow band between the interface of the fluids. When the distance function, ϕ, is calculated, the physical parameters, density and viscosity, are updated using the sign of ϕ. The jump in material properties between two fluids, such as air and water can be extreme, and so the transition of the properties from one medium to another is smoothed. The region of the interface is assumed to be of finite thickness of αh, where h is the size of the elements in the computational mesh and α is a smoothing parameter. The parameters are updated by the following expression:

$$P = \begin{cases} P_1 & where\ \ \psi < -\alpha h \\ P_2 & where\ \ \psi > \alpha h \\ (P_2 - P_1)\psi/2\alpha h + (P_1 + P_2)/2 & where\ \ |\psi| < \alpha h. \end{cases} \tag{2.83}$$

where the subscripts 1 and 2 denote the different fluids. The procedure of the level set calculation is shown in Figure 2.10. Further work is needed in the reinitialization procedure, as it has been shown that it is prone to mass loss and inconsistent positioning of the interface [14].

2.5.4 Benchmark Problem

The Rayleigh-Taylor instability problem is used as a benchmark to validate CFD implementations [16]. Figure 2.11 shows the setup of the problem. A rectangular domain with two different fluids is considered, with the greater density fluid on the top and the lighter density fluid on the bottom. The viscosities of the two fluids are equal (isoviscous). An initial perturbation is given to the interface of $\phi = 0.02cos(\frac{\pi x}{\lambda}) + 0.2$. The aspect ratio $\lambda = L/H = 0.9142$ is chosen such that it gives the greatest disturbance of the fluids.



Start
Initialize level set function
Solve Stokes equation for velocity and pressure
Solve the level set advection equation
Reinitialize the level set function
Update density and viscosity
$t = t_{end}$?
No
Yes
End
$t = t + \Delta t$

FIGURE 2.10: Flow chart of level set procedure [10].

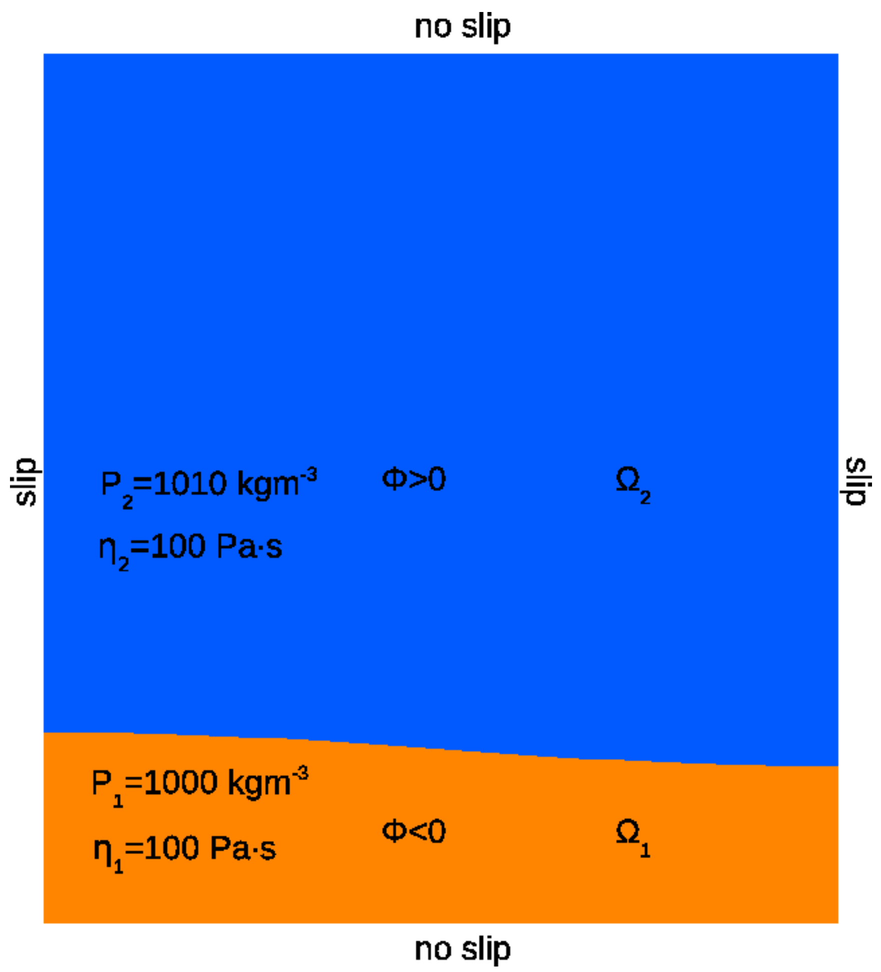


FIGURE 2.11: Parameters, initial interface and boundary conditions for the Rayleigh-Taylor instability problem. The interface is defined as $\phi = 0.02cos(\frac{\pi x}{\lambda}) + 0.2$. The fluids have been assigned different densities and equal viscosity (isoviscous) [7].

```
from esys.escript import *
import esys.finley
from esys.escript.models import StokesProblemCartesian
from esys.finley import finley
from LevelSet import *

#physical properties
rho1 = 1000             #fluid density on bottom
rho2 = 1010             #fluid density on top
eta1 = 100.0            #fluid viscosity on bottom
eta2 = 100.0            #fluid viscosity on top
penalty = 100.0
g=10.0

#solver settings
dt = 0.001
t_step = 0
t_step_end = 2000
TOL = 1.0e-5
max_iter=400
verbose=True
useUzawa=True

#define mesh
l0=0.9142
l1=1.0
n0=100
n1=100

mesh=esys.finley.Rectangle(l0=l0, l1=l1, order=2, n0=n0, n1=n1)
#get mesh dimensions
numDim = mesh.getDim()
#get element size
h = Lsup(mesh.getSize())
print "element size",h

#level set parameters
tolerance = 1.0e-6
reinit_max = 30
reinit_each = 3
alpha = 1
smooth = alpha*h

#boundary conditions
x = mesh.getX()
#left + bottom + right + top
b_c = whereZero(x[0])*[1.0,0.0] + whereZero(x[1])*[1.0,1.0] + whereZero(x[0]-l0)*[1.0,0.0] + whereZer

velocity = Vector(0.0, ContinuousFunction(mesh))
pressure = Scalar(0.0, ContinuousFunction(mesh))
Y = Vector(0.0,Function(mesh))

#define initial interface between fluids
xx = mesh.getX()[0]
yy = mesh.getX()[1]
func = Scalar(0.0, ContinuousFunction(mesh))
h_interface = Scalar(0.0, ContinuousFunction(mesh))
h_interface = h_interface + (0.02*cos(math.pi*xx/l0) + 0.2)
func = yy - h_interface
func_new = func.interpolate(ReducedSolution(mesh))

#Stokes cartesian
```

```
solution=StokesProblemCartesian(mesh,debug=True)
solution.setTolerance(TOL)
solution.setSubProblemTolerance(TOL**2)

#level set
levelset = LevelSet(mesh, func_new, reinit_max, reinit_each, tolerance, smooth)

while t_step <= t_step_end:
  #update density and viscosity
  rho = levelset.update_parameter(rho1, rho2)
  eta = levelset.update_parameter(eta1, eta2)

  #get velocity and pressue of fluid
  Y[1] = -rho*g
  solution.initialize(fixed_u_mask=b_c,eta=eta,f=Y)
  velocity,pressure=solution.solve(velocity,pressure,max_iter=max_iter,verbose=verbose,useUzawa=useU

  #update the interface
  func = levelset.update_phi(velocity, dt, t_step)

  print "##########################################################"
  print "time step:", t_step, " completed with dt:", dt
  print "Velocity: min =", inf(velocity), "max =", Lsup(velocity)
  print "##########################################################"

  #save interface, velocity and pressure
  saveVTK("phi2D.%2.4i.vtu"%t_step,interface=func,velocity=velocity,pressure=pressure)
  #courant condition
  dt = 0.4*Lsup(mesh.getSize())/Lsup(velocity)
  t_step += 1
```

CHAPTER

THREE

The Module `esys.escript`

`esys.escript` is a Python module that allows you to represent the values of a function at points in a `Domain` in such a way that the function will be useful for the Finite Element Method (FEM) simulation. It also provides what we call a function space that describes how the data is used in the simulation. Stored along with the data is information about the elements and nodes which will be used by `esys.finley`.

In order to understand what we mean by the term 'function space', consider that the solution of a partial differential equation (PDE) is a function on a domain Ω. When solving a PDE using FEM, the solution is piecewise-differentiable but, in general, its gradient is discontinuous. To reflect these different degrees of smoothness, different function spaces are used. For instance, in FEM, the displacement field is represented by its values at the nodes of the mesh, and so is continuous. The strain, which is the symmetric part of the gradient of the displacement field, is stored on the element centers, and so is considered to be discontinuous.

A function space is described by a `FunctionSpace` object. The following statement generates the object *solution_space* which is a `FunctionSpace` object and provides access to the function space of PDE solutions on the `Domain` *mydomain*:

```
solution_space=Solution(mydomain)
```

The following generators for function spaces on a `Domain` *mydomain* are available:

- *Solution(mydomain)*: solutions of a PDE.
- *ReducedSolution(mydomain)*: solutions of a PDE with a reduced smoothness requirement.
- *ContinuousFunction(mydomain)*: continuous functions, eg. a temperature distribution.
- *Function(mydomain)*: general functions which are not necessarily continuous, eg. a stress field.
- *FunctionOnBoundary(mydomain)*: functions on the boundary of the domain, eg. a surface pressure.
- *FunctionOnContact0(mydomain)*: functions on side 0 of the discontinuity.
- *FunctionOnContact1(mydomain)*: functions on side 1 of the discontinuity.

The reduced smoothness for PDE solution is often used to fulfill the Ladyzhenskaya-Babuska-Brezzi condition [**?**] when solving saddle point problems , eg. the Stokes equation. A discontinuity is a region within the domain across which functions may be discontinuous. The location of discontinuity is defined in the `Domain` object. Figure 3.1 shows the dependency between the types of function spaces in Finley (other libraries may have different relationships).

The solution of a PDE is a continuous function. Any continuous function can be seen as a general function on the domain and can be restricted to the boundary as well as to one side of discontinuity (the result will be different depending on which side is chosen). Functions on any side of the discontinuity can be seen as a function on the corresponding other side.

A function on the boundary or on one side of the discontinuity cannot be seen as a general function on the domain as there are no values defined for the interior. For most PDE solver libraries the space of the solution and continuous functions is identical, however in some cases, eg. when periodic boundary conditions are used in `esys.finley`, a solution fulfills periodic boundary conditions while a continuous function does not have to be periodic.

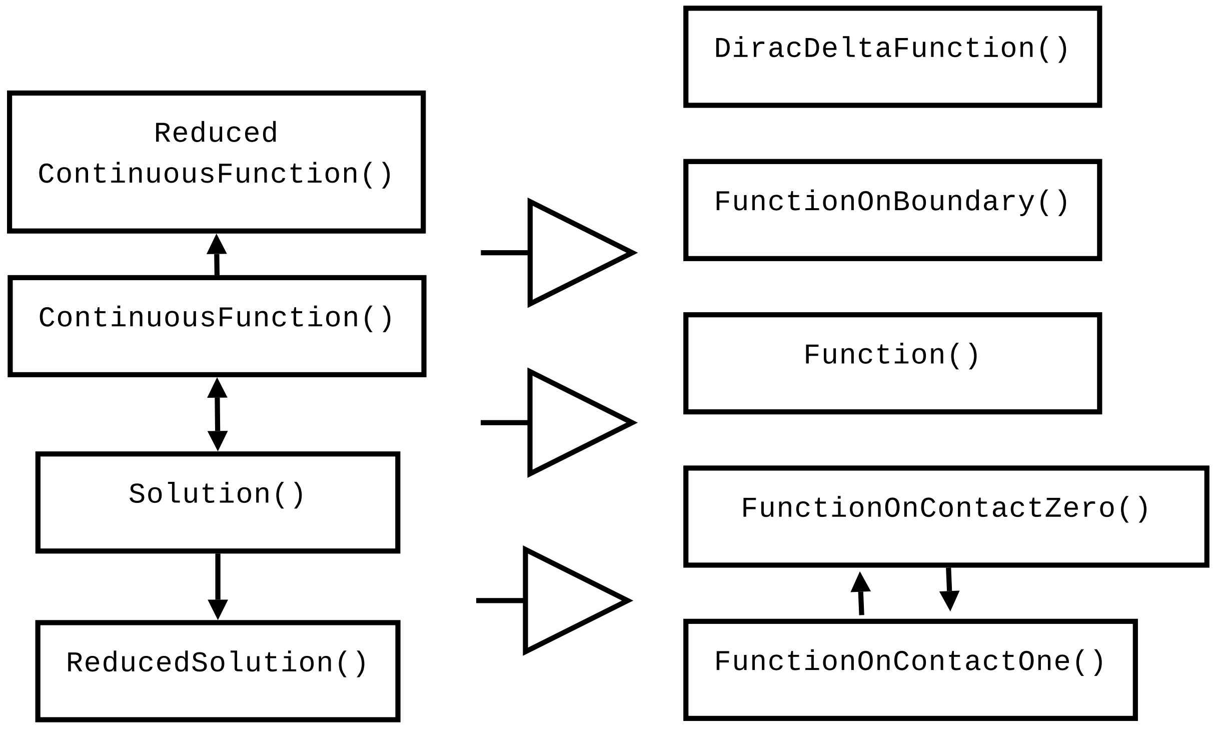


FIGURE 3.1: Dependency of Function Spaces in Finley. An arrow indicates that a function in the function space at the starting point can be interpolated to the function space of the arrow target. All functionspaces on the left side can be interpolated to any of the functionspaces on the right.

The concept of function spaces describes the properties of functions and allows abstraction from the actual representation of the function in the context of a particular application. For instance, in the FEM context a function of the general `FunctionSpace` type (written as *Function()* in Figure 3.1) is usually represented by its values at the element center, but in a finite difference scheme the edge midpoint of cells is preferred. By changing its function space you can use the same function in a Finite Difference scheme instead of Finite Element scheme. Changing the function space of a particular function will typically lead to a change of its representation. So, when seen as a general function, a continuous function which is typically represented by its values on the node of the FEM mesh or finite difference grid must be interpolated to the element centers or the cell edges, respectively. Interpolation happens automatically in `esys.escript` whenever it is required.

In `esys.escript` the class that stores these functions is called `Data`. The function is represented through its values on data sample points where the data sample points are chosen according to the function space of the function. `Data` class objects are used to define the coefficients of the PDEs to be solved by a PDE solver library and also to store the solutions of the PDE.

The values of the function have a rank which gives the number of indices, and a shape defining the range of each index. The rank in `esys.escript` is limited to the range 0 through 4 and it is assumed that the rank and shape is the same for all data sample points. The shape of a `Data` object is a tuple (list) *s* of integers. The length of *s* is the rank of the `Data` object and the *i*-th index ranges between 0 and *s[i]* -1. For instance, a stress field has rank 2 and shape (d,d) where d is the spatial dimension. The following statement creates the `Data` object *mydat* representing a continuous function with values of shape $(2,3)$ and rank 2:

```
mydat=Data(value=1,what=ContinuousFunction(myDomain),shape=(2,3))
```

The initial value is the constant 1 for all data sample points and all components.

`Data` objects can also be created from any `numarray` array or any object, such as a list of floating point numbers, that can be converted into a `numarray.NumArray` [11]. The following two statements create objects which are equivalent to *mydat*:

```
mydat1=Data(value=numarray.ones((2,3)),what=ContinuousFunction(myDomain))
mydat2=Data(value=[[1,1],[1,1],[1,1]],what=ContinuousFunction(myDomain))
```

In the first case the initial value is *numarray.ones((2,3))* which generates a 2×3 matrix as a numarray.NumArray filled with ones. The shape of the created Data object it taken from the shape of the array. In the second case, the creator converts the initial value, which is a list of lists, and converts it into a numarray.NumArray before creating the actual Data object.

For convenience esys.escript provides creators for the most common types of Data objects in the following forms (*d* defines the spatial dimension):

- *Scalar(0,Function(mydomain))* is the same as *Data(0,Function(myDomain),(,))* (each value is a scalar), e.g a temperature field.
- *Vector(0,Function(mydomain))* is the same as *Data(0,Function(myDomain),(d))* (each value is a vector), e.g a velocity field.
- *Tensor(0,Function(mydomain))* is the same as *Data(0,Function(myDomain),(d,d))*, eg. a stress field.
- *Tensor4(0,Function(mydomain))* is the same as *Data(0,Function(myDomain),(d,d,d,d))* eg. a Hook tensor field.

Here the initial value is 0 but any object that can be converted into a numarray.NumArray and whose shape is consistent with shape of the Data object to be created can be used as the initial value.

Data objects can be manipulated by applying unary operations (eg. cos, sin, log) point and can be combined point-wise by applying arithmetic operations (eg. +, - ,* , /). It is to be emphasized that esys.escript itself does not handle any spatial dependencies as it does not know how values are interpreted by the processing PDE solver library. However esys.escript invokes interpolation if this is needed during data manipulations. Typically, this occurs in binary operation when both arguments belong to different function spaces or when data are handed over to a PDE solver library which requires functions to be represented in a particular way.

The following example shows the usage of Data objects: Assume we have a displacement field u and we want to calculate the corresponding stress field σ using the linear–elastic isotropic material model

$$\sigma_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i}) \tag{3.1}$$

where δ_{ij} is the Kronecker symbol and λ and μ are the Lame coefficients. The following function takes the displacement u and the Lame coefficients *lam* and *mu* as arguments and returns the corresponding stress:

```
from esys.escript import *
def getStress(u,lam,mu):
  d=u.getDomain().getDim()
  g=grad(u)
  stress=lam*trace(g)*kronecker(d)+mu*(g+transpose(g))
  return stress
```

The variable *d* gives the spatial dimension of the domain on which the displacements are defined. *kronecker* returns the Kronecker symbol with indexes i and j running from 0 to *d*-1. The call *grad(u)* requires the displacement field *u* to be in the *Solution* or continuous FunctionSpace function space. The result *g* as well as the returned stress will be in the general FunctionSpace function space. If, for example, *u* is the solution of a PDE then *getStress* might be called in the following way:

```
s=getStress(u,1.,2.)
```

However *getStress* can also be called with Data objects as values for *lam* and *mu* which, for instance in the case of a temperature dependency, are calculated by an expression. The following call is equivalent to the previous example:

```
lam=Scalar(1.,ContinuousFunction(mydomain))
mu=Scalar(2.,Function(mydomain))
s=getStress(u,lam,mu)
```

The function *lam* belongs to the continuous FunctionSpace function space but with *g* the function *trace(g)* is in the general FunctionSpace function space. In the evaluation of the product *lam*trace(g)* we have different function spaces (on the nodes versus in the centers) and at first glance we have incompatible data. esys.escript converts the arguments in an appropriate function space according to Table 3.1. In this example that means esys.escript sees *lam* as a function of the general FunctionSpace function space. In

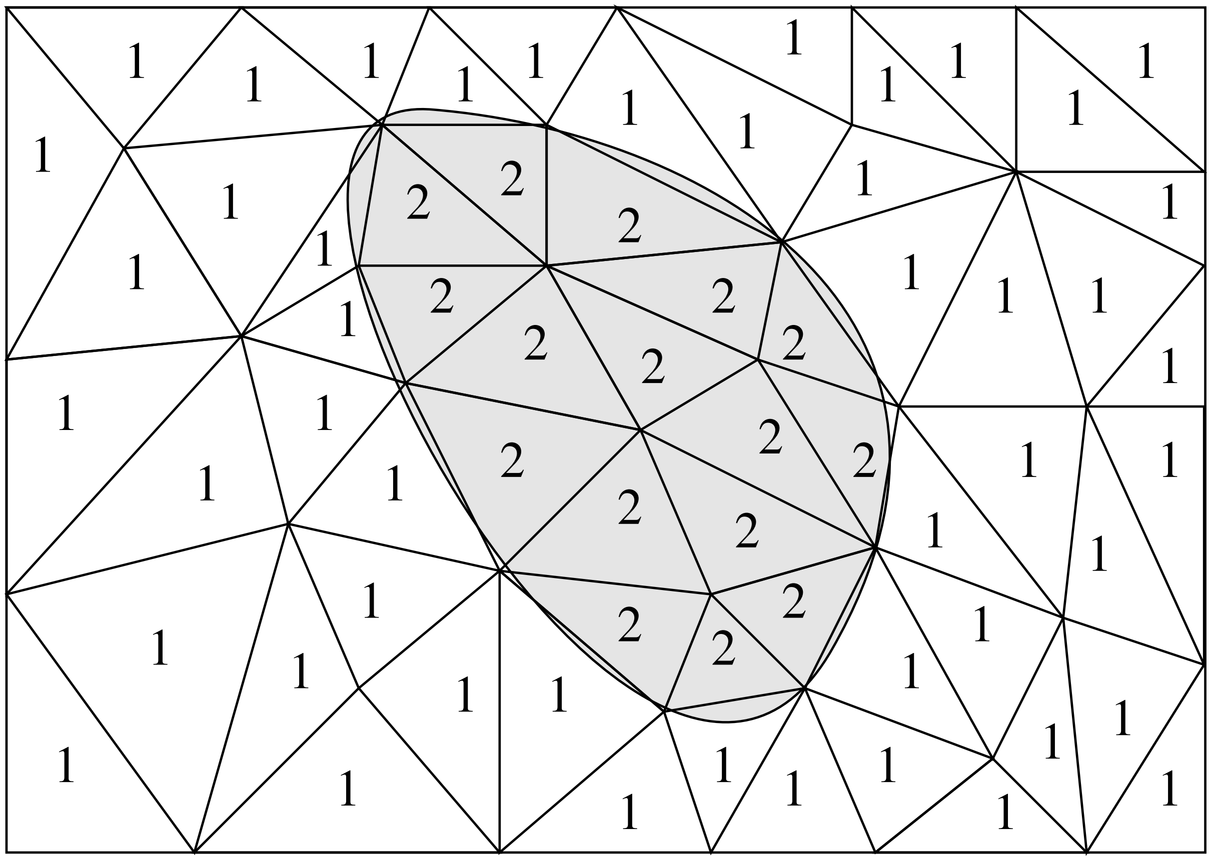


FIGURE 3.2: Element Tagging. A rectangular mesh over a region with two rock types *white* and *gray*. The number in each cell refers to the major rock type present in the cell (1 for *white* and 2 for *gray*).

the context of FEM this means the nodal values of *lam* are interpolated to the element centers. The interpolation is automatic and requires no special handling.

Material parameters such as the Lame coefficients are typically dependent on rock types present in the area of interest. A common technique to handle these kinds of material parameters is ”tagging”, which uses storage efficiently. Figure 3.2 shows an example. In this case two rock types *white* and *gray* can be found in the domain. The domain is subdivided into triangular shaped cells. Each cell has a tag indicating the rock type predominately found in this cell. Here 1 is used to indicate rock type *white* and 2 for rock type *gray*. The tags are assigned at the time when the cells are generated and stored in the `Domain` class object. To allow easier usage of tags, names can be used instead of numbers. These names are typically defined at the time when the geometry is generated.

The following statements show how, for the example of Figure 3.2, the stress calculation discussed above and tagged values are used for *lam*:

```
lam=Scalar(value=2.,what=Function(mydomain))
insertTaggedValue(lam,white=30.,gray=5000.)
s=getStress(u,lam,2.)
```

In this example *lam* is set to 30 for those cells with tag *white* (=1) and to 5000. for those cells with tag *gray* (=2_. The initial value 2 of *lam* is used as a default value for the case when a tag is encountered which has not been linked with a value. The *getStress* method does not need to be changed now that we are using tags. `esys.escript` resolves the tags when *lam*trace(g)* is calculated.

This brings us to a very important point about `esys.escript`. You can develop a simulation with constant Lame coefficients, and then later switch to tagged Lame coefficients without otherwise changing your python script. In short, you can use the same script to model with different domains and different types of input data.

There are three main ways in which `Data` objects are represented internally: constant, tagged, and expanded. In the constant case, the same value is used at each sample point and only a single value is stored to save memory. In the expanded case, each sample point has an individual value (such as for the solution of a PDE). This is where your largest data sets will be created because the values are stored as a complete array. The tagged case has already been discussed above.

Expanded data is created when you create a `Data` object with expanded=True. Tagged data sets are created when you use the insertTaggedValue() method as shown above.

Values are accessed through a sample reference number. Operations on expanded `Data` objects have to be performed for each sample point individually. When tagged values are used, the values are held in a dictionary. Operations on tagged data require processing the set of tagged values only, rather than processing the value for each individual sample point. `esys.escript` allows any mixture of constant, tagged and expanded data in a single expression.

`Data` objects can be written to disk files and read with *dump* and *load*, both of which use *netCDF*[3] . Use these to save data for visualization, checkpoint/restart or simply to save and reuse data that was expensive to compute.

For instance to save the coordinates of the data points of the continuous `FunctionSpace` to the file `x.nc` use

```
x=ContinuousFunction(mydomain).getX()
x.dump("x.nc")
```

To recover the object *x* use

```
x=load("x.nc", mydomain)
```

The dump file `x.nc` does not contain a representation of the `Domain`, even though it is required to recreate *x*. It is common to simply recreate the `Domain` before reading a `Data`, or you may read and write your `Domain` in a separate file with *domain=ReadMesh(fileName)* and *domain.write(fileName)*.

The function space of the `Data` is stored in `x.nc`, though. If the `Data` object is expanded, the number of data points in the file and of the `Domain` for the particular `FunctionSpace` must match. Moreover, the ordering of the values is checked using the reference identifiers provided by `FunctionSpace` on the `Domain`. In some cases, data points will be re-ordered. Take care to be sure you get what you want!

3.1 `esys.escript` Classes

3.1.1 `Domain` class

class `Domain`( )

A `Domain` object is used to describe a geometric region together with a way of representing functions over this region. The `Domain` class provides an abstract interface to the domain of `FunctionSpace` and `Data` objects. `Domain` needs to be subclassed in order to provide a complete implementation.

The following methods are available:

`getDim`( )

returns the spatial dimension of the `Domain`.

`getX`( )

returns the locations in the `Domain`. The `FunctionSpace` of the returned `Data` object is chosen by the `Domain` implementation. Typically it will be in the general `FunctionSpace`.

`setX`(*newX*)

assigns a new location to the `Domain`. *newX* has to have shape $(d,)$ where d is the spatial dimension of the domain. Typically *newX* must be in the continuous `FunctionSpace` but the space actually to be used depends on the `Domain` implementation.

`getNormal`( )

returns the surface normals on the boundary of the `Domain` as `Data` object.

`getSize`( )

returns the local sample size, e.g. the element diameter, as `Data` object.

`setTagMap`(*tag_name, tag*)

defines a mapping of the tag name *tag_name* to the *tag*.

getTag(*tag_name*)
returns the tag associated with the tag name *tag_name*.

isValidTagName(*tag_name*)
return `True` if *tag_name* is a valid tag name.

__eq__(*arg*)
(python == operator) returns `True` if the `Domain` *arg* describes the same domain. Otherwise `False` is returned.

__ne__(*arg*)
(python != operator) returns `True` if the `Domain` *arg* does not describe the same domain. Otherwise `False` is returned.

__str__(*arg*)
(python str() function) returns string representation of the `Domain`.

onMasterProcessor()
returns `True` if executed on the MPI master processor, `False` otherwise. This can be used in conjunction with MPIBarrier to ensure commands only run once.

MPIBarrier()
executes an MPIBarrier command. If MPI support is not enabled, this command does nothing.

MPIBarrier()
executes an MPIBarrier command. If MPI support is not enabled, this command does nothing.

getMPISize()
returns the number of MPI processors used for this domain.

getMPIRank()
returns the rank of the processor executing the statement.

3.1.2 `FunctionSpace` class

class FunctionSpace()
`FunctionSpace` objects are used to define properties of `Data` objects, such as continuity. `FunctionSpace` objects are instantiated by generator functions. A `Data` object in a particular `FunctionSpace` is represented by its values at data sample points which are defined by the type and the `Domain` of the `FunctionSpace`.

The following methods are available:

getDim()
returns the spatial dimension of the `Domain` of the `FunctionSpace`.

getX()
returns the location of the data sample points.

getNormal()
If the domain of functions in the `FunctionSpace` is a hypermanifold (e.g. the boundary of a domain) the method returns the outer normal at each of the data sample points. Otherwise an exception is raised.

getSize()
returns a `Data` objects measuring the spacing of the data sample points. The size may be zero.

getDomain()
returns the `Domain` of the `FunctionSpace`.

setTags(*new_tag, mask*)
assigns a new tag *new_tag* to all data sample where *mask* is positive for a least one data point. *mask* must be defined on the this `FunctionSpace`. Use the *setTagMap* to assign a tag name to *new_tag*.

__eq__(*arg*)
(python == operator) returns `True` if the `Domain` *arg* describes the same domain. Otherwise `False` is returned.

`__ne__`(*arg*)
: (python != operator) returns `True` if the `Domain` *arg* do not describe the same domain. Otherwise `False` is returned.

`__str__`(*g*)
: (python str() function) returns string representation of the `Domain`.

The following function provide generators for `FunctionSpace` objects:

`Function`(*domain*)
: returns the general `FunctionSpace` on the `Domain` *domain*. `Data` objects in this type of general `FunctionSpace` are defined over the whole geometric region defined by *domain*.

`ContinuousFunction`(*domain*)
: returns the continuous `FunctionSpace` on the `Domain` domain. `Data` objects in this type of general `FunctionSpace` are defined over the whole geometric region defined by *domain* and assumed to represent a continuous function.

`FunctionOnBoundary`(*domain*)
: returns the continuous `FunctionSpace` on the `Domain` domain. `Data` objects in this type of general `FunctionSpace` are defined on the boundary of the geometric region defined by *domain*.

`FunctionOnContactZero`(*domain*)
: returns the contact `FunctionSpace` on side 0 the `Domain` domain. `Data` objects in this type of general `FunctionSpace` are defined on side 0 of a discontinuity within the geometric region defined by *domain*. The discontinuity is defined when *domain* is instantiated.

`FunctionOnContactOne`(*domain*)
: returns the contact `FunctionSpace` on side 1 on the `Domain` domain. `Data` objects in this type of general `FunctionSpace` are defined on side 1 of a discontinuity within the geometric region defined by *domain*. The discontinuity is defined when *domain* is instantiated.

`Solution`(*domain*)
: returns the solution `FunctionSpace` on the `Domain` domain. `Data` objects in this type of general `FunctionSpace` are defined on geometric region defined by *domain* and are solutions of partial differential equations .

`ReducedSolution`(*domain*)
: returns the reduced solution `FunctionSpace` on the `Domain` domain. `Data` objects in this type of general `FunctionSpace` are defined on geometric region defined by *domain* and are solutions of partial differential equations with a reduced smoothness for the solution approximation.

3.1.3 `Data` Class

The following table shows arithmetic operations that can be performed point-wise on `Data` objects.

expression	**Description**
+*arg0*	identical to *arg*
-*arg0*	negation
arg0+*arg1*	adds *arg0* and *arg1*
*arg0***arg1*	multiplies *arg0* and *arg1*
arg0-*arg1*	difference *arg1* from*arg1*
arg0/*arg1*	divide *arg0* by *arg1*
*arg0****arg1*	raises *arg0* to the power of *arg1*

At least one of the arguments *arg0* or *arg1* must be a `Data` object. Either of the arguments may be a `Data` object, a python number or a numarray object.

If *arg0* or *arg1* are not defined on the same `FunctionSpace`, then an attempt is made to convert *arg0* to the `FunctionSpace` of *arg1* or to convert *arg1* to the `FunctionSpace` of *arg0*. Both arguments must have the same shape or one of the arguments may be of rank 0 (a constant).

The returned `Data` object has the same shape and is defined on the data sample points as *arg0* or *arg1*.

The following table shows the update operations that can be applied to `Data` objects:

expression	Description
arg0+=arg2	adds *arg0* to *arg2*
arg0=arg2*	multiplies *arg0* with *arg2*
arg0-=arg2	subtracts *arg2* from*arg2*
arg0/=arg2	divides *arg0* by *arg2*
*arg0**=arg2*	raises *arg0* by *arg2*

arg0 must be a `Data` object. *arg1* must be a `Data` object or an object that can be converted into a `Data` object. *arg1* must have the same shape as *arg0* or have rank 0. In the latter case it is assumed that the values of *arg1* are constant for all components. *arg1* must be defined in the same `FunctionSpace` as *arg0* or it must be possible to interpolate *arg1* onto the `FunctionSpace` of *arg0*.

The `Data` class supports taking slices from a `Data` object as well as assigning new values to a slice of an existing `Data` object. The following expressions for taking and setting slices are valid:

rank of *arg*	slicing expression	shape of returned and assigned object
0	no slicing	-
1	*arg[l0:u0]*	(*u0-l0*,)
2	*arg[l0:u0,l1:u1]*	(*u0-l0*,*u1-l1*)
3	*arg[l0:u0,l1:u1,l2:u2]*	(*u0-l0*,*u1-l1*,*u2-l2*)
4	*arg[l0:u0,l1:u1,l2:u2,l3:u3]*	(*u0-l0*,*u1-l1*,*u2-l2*,*u3-l3*)

where *s* is the shape of *arg* and

$$0 \le l0 \le u0 \le s[0],$$

$$0 \le l1 \le u1 \le s[1],$$

$$0 \le l2 \le u2 \le s[2],$$

$$0 \le l3 \le u3 \le s[3].$$

Any of the lower indexes *l0*, *l1*, *l2* and *l3* may not be present in which case 0 is assumed. Any of the upper indexes *u0*, *u1*, *u2* and *u3* may be ommitted, in which case, the upper limit for that dimension is assumed. The lower and upper index may be identical, in which case the column and the lower or upper index may be dropped. In the returned or in the object assigned to a slice, the corresponding component is dropped, i.e. the rank is reduced by one in comparison to *arg*. The following examples show slicing in action:

```
t=Data(1.,(4,4,6,6),Function(mydomain))
t[1,1,1,0]=9.
s=t[:2,:,2:6,5] # s has rank 3
s[:,:,1]=1.
t[:2,:2,5,5]=s[2:4,1,:2]
```

3.1.4 Generation of `Data` objects

class `Data`(*value=0,shape=(,),what=FunctionSpace(),expand=*`False`)

creates a `Data` object with shape *shape* in the `FunctionSpace` *what*. The values at all data sample points are set to the double value *value*. If *expanded* is `True` the `Data` object is represented in expanded from.

class `Data`(*value,what=FunctionSpace(),expand=*`False`)

creates a `Data` object in the `FunctionSpace` *what*. The value for each data sample points is set to *value*, which could be a `numarray`, `Data` object *value* or a dictionary of `numarray` or floating point numbers. In the latter case the keys must be integers and are used as tags. The shape of the returned object is equal to the shape of *value*. If *expanded* is `True` the `Data` object is represented in expanded form.

class `Data`()

creates an empty `Data` object. The empty `Data` object is used to indicate that an argument is not present where a `Data` object is required.

Scalar(*value=0.,what=FunctionSpace(),expand=*`False`)
: returns a `Data` object of rank 0 (a constant) in the `FunctionSpace` *what*. Values are initialised with *value*, a double precision quantity. If *expanded* is `True` the `Data` object is represented in expanded from.

Vector(*value=0.,what=FunctionSpace(),expand=*`False`)
: returns a `Data` object of shape *(d,)* in the `FunctionSpace` *what*, where *d* is the spatial dimension of the `Domain` of *what*. Values are initialed with *value*, a double precision quantity. If *expanded* is `True` the `Data` object is represented in expanded from.

Tensor(*value=0.,what=FunctionSpace(),expand=*`False`)
: returns a `Data` object of shape *(d,d)* in the `FunctionSpace` *what*, where *d* is the spatial dimension of the `Domain` of *what*. Values are initialed with *value*, a double precision quantity. If *expanded* is `True` the `Data` object is represented in expanded from.

Tensor3(*value=0.,what=FunctionSpace(),expand=*`False`)
: returns a `Data` object of shape *(d,d,d)* in the `FunctionSpace` *what*, where *d* is the spatial dimension of the `Domain` of *what*. Values are initialed with *value*, a double precision quantity. If *expanded* is `True` the `Data` object is re*arg*presented in expanded from.

Tensor4(*value=0.,what=FunctionSpace(),expand=*`False`)
: returns a `Data` object of shape *(d,d,d,d)* in the `FunctionSpace` *what*, where *d* is the spatial dimension of the `Domain` of *what*. Values are initialised with *value*, a double precision quantity. If *expanded* is `True` the `Data` object is represented in expanded from.

load(*filename,domain*)
: recovers a `Data` object on `Domain` *domain* from the file *filename*, which was created by *dump*.

3.1.5 `Data` methods

These are the most frequently-used methods of the `Data` class. A complete list of methods can be found on http://shake200.esscc.uq.edu.au/esys/esys13/release/epydoc/index.html.

getFunctionSpace()
: returns the `FunctionSpace` of the object.

getDomain()
: returns the `Domain` of the object.

getShape()
: returns the shape of the object as a `tuple` of integers.

getRank()
: returns the rank of the data on each data point.

isEmpty()
: returns `True` id the `Data` object is the empty `Data` object. Otherwise `False` is returned. Note that this is not the same as asking if the object contains no data sample points.

setTaggedValue(*tag_name,value*)
: assigns the *value* to all data sample points which have the tag assigned to *tag_name*. *value* must be an object of class `numarray.NumArray` or must be convertible into a `numarray.NumArray` object. *value* (or the corresponding `numarray.NumArray` object) must be of rank 0 or must have the same rank like the object. If a value has already be defined for tag *tag_name* within the object it is overwritten by the new *value*. If the object is expanded, the value assigned to data sample points with tag *tag_name* is replaced by *value*. If no tag is assigned tag name *tag_name*, no value is set.

dump(*filename*)
: dumps the `Data` object to the file *filename*. The file stores the function space but not the `Domain`. It is in the responsibility of the user to save the `Domain`.

__str__()
: returns a string representation of the object.

3.1.6 Functions of `Data` objects

This section lists the most important functions for `Data` class objects *a*. A complete list and a more detailed description of the functionality can be found on http://shake200.esscc.uq.edu.au/esys/esys13/release/epydoc/index.html.

`saveVTK`(*filename*,***kwdata*)
writes `Data` defined by keywords in the file with *filename* using the vtk file format *VTK* file format. The key word is used as an identifier. The statement

```
saveVTK("out.xml",temperature=T,velocity=v)
```

will write the scalar *T* as *temperature* and the vector *v* as *velocity* into the file 'out.xml'. Restrictions on the allowed combinations of `FunctionSpace` apply.

`saveDX`(*filename*,***kwdata*)
writes `Data` defined by keywords in the file with *filename* using the vtk file format *OpenDX* [4] file format. The key word is used as an identifier. The statement

```
saveDX("out.dx",temperature=T,velocity=v)
```

will write the scalar *T* as *temperature* and the vector *v* as *velocity* into the file 'out.dx'. Restrictions on the allowed combinations of `FunctionSpace` apply.

`kronecker`(*d*)
returns a rank-2 `Data` object `Data` object in `FunctionSpace` *d* such that

$$\texttt{kronecker(d)}[i,j] = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \tag{3.2}$$

If *d* is an integer a (d,d) `numarray` array is returned.

`identityTensor`(*d*)
is a synonym for `kronecker` (see above).

`identityTensor4`(*d*)
returns a rank-4 `Data` object `Data` object in `FunctionSpace` *d* such that

$$\texttt{identityTensor(d)}[i,j,k,l] = \begin{cases} 1 & \text{if } i = k \text{ and } j = l \\ 0 & \text{otherwise} \end{cases} \tag{3.3}$$

If *d* is an integer a (d,d,d,d) `numarray` array is returned.

`unitVector`(*i*,*d*)
returns a rank-1 `Data` object `Data` object in `FunctionSpace` *d* such that

$$\texttt{identityTensor(d)}[j] = \begin{cases} 1 & \text{if } j = i \\ 0 & \text{otherwise} \end{cases} \tag{3.4}$$

If *d* is an integer a $(d,)$ `numarray` array is returned.

`Lsup`(*a*)
returns the L^{sup} norm of *arg*. This is the maximum of the absolute values over all components and all data sample points of *a*.

`sup`(*a*)
returns the maximum value over all components and all data sample points of *a*.

`inf`(*a*)
returns the minimum value over all components and all data sample points of *a*

`minval`(*a*)
returns at each data sample points the minimum value over all components.

`maxval`(*a*)
returns at each data sample points the maximum value over all components.

length(a)

returns at Euclidean norm at each data sample points. For a rank-4 `Data` object a this is

$$\texttt{length(a)} = \sqrt{\sum_{ijkl} a\left[i,j,k,l\right]^2} \tag{3.5}$$

trace(a[,$axis\_offset$=0])

returns the trace of a. This is the sum over components *axis_offset* and *axis_offset+1* with the same index. For instance in the case of a rank-2 `Data` object function and this is

$$\texttt{trace(a)} = \sum_i a\left[i,i\right] \tag{3.6}$$

and for a rank-4 `Data` object function and `axis_offset=1` this is

$$\texttt{trace(a,1)}\left[i,j\right] = \sum_k a\left[i,k,k,j\right] \tag{3.7}$$

transpose(a[, $axis\_offset$=None])

returns the transpose of a. This swaps the first *axis_offset* components of a with the rest. If *axis_offset* is not present `int(r/2)` is used where r is the rank of a. the sum over components *axis_offset* and *axis_offset+1* with the same index. For instance in the case of a rank-2 `Data` object function and this is

$$\texttt{transpose(a)}\left[i,j\right] = a\left[j,i\right] \tag{3.8}$$

and for a rank-4 `Data` object function and `axis_offset=1` this is

$$\texttt{transpose(a,1)}\left[i,j,k,l\right] = a\left[j,k,l,i\right] \tag{3.9}$$

swap_axes(a[, $axis0$=0 [, $axis1$=1]])

returns a but with swapped components *axis0* and *axis1*. The argument a must be at least of rank-2 `Data` object. For instance in the for a rank-4 `Data` object argument, `axis0=1` and `axis1=2` this is

$$\texttt{swap\_axes(a,1,2)}\left[i,j,k,l\right] = a\left[i,k,j,l\right] \tag{3.10}$$

symmetric(a)

returns the symmetric part of a. This is `(a+transpose(a))/2`.

nonsymmetric(a)

returns the non–symmetric part of a. This is `(a-transpose(a))/2`.

inverse(a)

return the inverse of a. This is

$$\texttt{matrix\_mult(inverse(a),a)=kronecker(d)} \tag{3.11}$$

if a has shape `(d,d)`. The current implementation is restricted to arguments of shape `(2,2)` and `(3,3)`.

eigenvalues(a)

return the eigenvalues of a. This is

$$\texttt{matrix\_mult(a,V)=e[i]*V} \tag{3.12}$$

where `e=eigenvalues(a)` and V is suitable non–zero vector V. The eigenvalues are ordered in increasing size. The argument a has to be the symmetric, ie. `a=symmetric(a)`. The current implementation is restricted to arguments of shape `(2,2)` and `(3,3)`.

eigenvalues_and_eigenvectors(a)

return the eigenvalues and eigenvectors of a. This is

$$\texttt{matrix\_mult(a,V[:,i])=e[i]*V[:,i]} \tag{3.13}$$

where `e,V=eigenvalues_and_eigenvectors(a)`. The eigenvectors V are orthogonal and normalized, ie.

$$\texttt{matrix\_mult(transpose(V),V)=kronecker(d)} \tag{3.14}$$

if a has shape `(d,d)`. The eigenvalues are ordered in increasing size. The argument a has to be the symmetric, ie. `a=symmetric(a)`. The current implementation is restricted to arguments of shape `(2,2)` and `(3,3)`.

maximum(**a*)
returns the maximum value over all arguments at all data sample points and for each component. For instance

$$\texttt{maximum(a0,a1)}[i,j] = max(\textit{a0}[i,j], \textit{a1}[i,j]) \tag{3.15}$$

at all data sample points.

minimum(**a*)
returns the minimum value over all arguments at all data sample points and for each component. For instance

$$\texttt{minimum(a0,a1)}[i,j] = min(\textit{a0}[i,j], \textit{a1}[i,j]) \tag{3.16}$$

at all data sample points.

clip(*a*[*, minval=0.*][*, maxval=1.*])
cuts back *a* into the range between *minval* and *maxval*. A value in the returned object equals *minval* if the corresponding value of *a* is less than *minval*, equals *maxval* if the corresponding value of *a* is greater than *maxval* or corresponding value of *a* otherwise.

inner(*a0,a1*)
returns the inner product of *a0* and *a1*. For instance in the case of rank-2 `Data` object arguments and this is

$$\texttt{inner(a)} = \sum_{ij} \textit{a0}[j,i] \cdot \textit{a1}[j,i] \tag{3.17}$$

and for a rank-4 `Data` object arguments this is

$$\texttt{inner(a)} = \sum_{ijkl} \textit{a0}[i,j,k,l] \cdot \textit{a1}[j,i,k,l] \tag{3.18}$$

matrix_mult(*a0,a1*)
returns the matrix product of *a0* and *a1*. If *a1* is rank-1 `Data` object this is

$$\texttt{matrix\_mult(a)}[i] = \sum_{k} \textit{a0} \cdot [i,k]\,\textit{a1}[k] \tag{3.19}$$

and if *a1* is rank-2 `Data` object this is

$$\texttt{matrix\_mult(a)}[i,j] = \sum_{k} \textit{a0} \cdot [i,k]\,\textit{a1}[k,j] \tag{3.20}$$

transposed_matrix_mult(*a0,a1*)
returns the matrix product of the transposed of *a0* and *a1*. The function is equivalent to `matrix_mult(transpose(a0),a1)`. If *a1* is rank-1 `Data` object this is

$$\texttt{transposed\_matrix\_mult(a)}[i] = \sum_{k} \textit{a0} \cdot [k,i]\,\textit{a1}[k] \tag{3.21}$$

and if *a1* is rank-2 `Data` object this is

$$\texttt{transposed\_matrix\_mult(a)}[i,j] = \sum_{k} \textit{a0} \cdot [k,i]\,\textit{a1}[k,j] \tag{3.22}$$

matrix_transposed_mult(*a0,a1*)
returns the matrix product of *a0* and the transposed of *a1*. The function is equivalent to `matrix_mult(a0,transpose(a1))`. If *a1* is rank-2 `Data` object this is

$$\texttt{matrix\_transposed\_mult(a)}[i,j] = \sum_{k} \textit{a0} \cdot [i,k]\,\textit{a1}[j,k] \tag{3.23}$$

outer(*a0,a1*)
returns the outer product of *a0* and *a1*. For instance if *a0* and *a1* both are rank-1 `Data` object then

$$\texttt{outer(a)}[i,j] = \textit{a0}[i] \cdot \textit{a1}[j] \tag{3.24}$$

and if *a0* is rank-1 `Data` object and *a1* is rank-3 `Data` object

$$\texttt{outer(a)}[i,j,k] = \textit{a0}[i] \cdot \textit{a1}[j,k] \tag{3.25}$$

`tensor_mult`(*a0*,*a1*)

returns the tensor product of *a0* and *a1*. If *a1* is rank-2 `Data` object this is

$$\texttt{tensor\_mult(a)}\,[i,j] = \sum_{kl} \mathit{a0}\,[i,j,k,l] \cdot \mathit{a1}\,[k,l] \tag{3.26}$$

and if *a1* is rank-4 `Data` object this is

$$\texttt{tensor\_mult(a)}\,[i,j,k,l] = \sum_{mn} \mathit{a0}\,[i,j,m,n] \cdot \mathit{a1}\,[m,n,k,l] \tag{3.27}$$

`transposed_tensor_mult`(*a0*,*a1*)

returns the tensor product of the transposed of *a0* and *a1*. The function is equivalent to `tensor_mult(transpose(a0),a1)`. If *a1* is rank-2 `Data` object this is

$$\texttt{transposed\_tensor\_mult(a)}\,[i,j] = \sum_{kl} \mathit{a0}\,[k,l,i,j] \cdot \mathit{a1}\,[k,l] \tag{3.28}$$

and if *a1* is rank-4 `Data` object this is

$$\texttt{transposed\_tensor\_mult(a)}\,[i,j,k,l] = \sum_{mn} \mathit{a0}\,[m,n,i,j] \cdot \mathit{a1}\,[m,n,k,l] \tag{3.29}$$

`tensor_transposed_mult`(*a0*,*a1*)

returns the tensor product of *a0* and the transposed of *a1*. The function is equivalent to `tensor_mult(a0,transpose(a1))`. If *a1* is rank-2 `Data` object this is

$$\texttt{tensor\_transposed\_mult(a)}\,[i,j] = \sum_{kl} \mathit{a0}\,[i,j,k,l] \cdot \mathit{a1}\,[l,k] \tag{3.30}$$

and if *a1* is rank-4 `Data` object this is

$$\texttt{tensor\_transposed\_mult(a)}\,[i,j,k,l] = \sum_{mn} \mathit{a0}\,[i,j,m,n] \cdot \mathit{a1}\,[k,l,m,n] \tag{3.31}$$

`grad`(*a*[, *where=None*])

returns the gradient of *a*. If *where* is present the gradient will be calculated in `FunctionSpace` *where* otherwise a default `FunctionSpace` is used. In case that *a* has rank-2 `Data` object one has

$$\texttt{grad(a)}\,[i,j,k] = \frac{\partial \mathit{a}\,[i,j]}{\partial x_k} \tag{3.32}$$

`integrate`(*a*[,*where=None*])

returns the integral of *a* where the domain of integration is defined by the `FunctionSpace` of *a*. If *where* is present the argument is interpolated into `FunctionSpace` *where* before integration. For instance in the case of a rank-2 `Data` object argument in continuous `FunctionSpace` it is

$$\texttt{integrate(a)}\,[i,j] = \int_{\Omega} \mathit{a}\,[i,j]\; d\Omega \tag{3.33}$$

where Ω is the spatial domain and $d\Omega$ volume integration. To integrate over the boundary of the domain one uses

$$\texttt{integrate(a,where=FunctionOnBoundary(a.getDomain))}\,[i,j] = \int_{\partial\Omega} a\,[i,j]\; ds \tag{3.34}$$

where $\partial\Omega$ is the surface of the spatial domain and ds area or line integration.

`interpolate`(*a*,*where*)

interpolates argument *a* into the `FunctionSpace` *where*.

`div`(*a*[,*where=None*])

returns the divergence of *a*. This

$$\texttt{div(a)} = trace(grad(a), where) \tag{3.35}$$

jump(*a*[*,domain=None*])
: returns the jump of *a* over the discontinuity in its domain or if `Domain` *domain* is present in *domain*.

$$\begin{aligned}\texttt{jump(a)} &= \texttt{interpolate(a,FunctionOnContactOne(domain))} \\ &\quad -\texttt{interpolate(a,FunctionOnContactZero(domain))}\end{aligned} \tag{3.36}$$

L2(*a*)
: returns the L^2-norm of *a* in its function space. This is

$$\texttt{L2(a)=integrate(length(a)}^2\texttt{)} . \tag{3.37}$$

The following functions operate "point-wise". That is, the operation is applied to each component of each point individually.

sin(*a*)
: applies sine function to *a*.

cos(*a*)
: applies cosine function to *a*.

tan(*a*)
: applies tangent function to *a*.

asin(*a*)
: applies arc (inverse) sine function to *a*.

acos(*a*)
: applies arc (inverse) cosine function to *a*.

atan(*a*)
: applies arc (inverse) tangent function to *a*.

sinh(*a*)
: applies hyperbolic sine function to *a*.

cosh(*a*)
: applies hyperbolic cosine function to *a*.

tanh(*a*)
: applies hyperbolic tangent function to *a*.

asinh(*a*)
: applies arc (inverse) hyperbolic sine function to *a*.

acosh(*a*)
: applies arc (inverse) hyperbolic cosine function to *a*.

atanh(*a*)
: applies arc (inverse) hyperbolic tangent function to *a*.

exp(*a*)
: applies exponential function to *a*.

sqrt(*a*)
: applies square root function to *a*.

log(*a*)
: applies the natural logarithm to *a*.

log10(*a*)
: applies the base-10 logarithm to *a*.

sign(*a*)
: applies the sign function to *a*, that is 1 where *a* is positive, -1 where *a* is negative and 0 otherwise.

wherePositive(*a*)
: returns a function which is 1 where *a* is positive and 0 otherwise.

whereNegative(*a*)
: returns a function which is 1 where *a* is negative and 0 otherwise.

whereNonNegative(*a*)
: returns a function which is 1 where *a* is non–negative and 0 otherwise.

whereNonPositive(*a*)
: returns a function which is 1 where *a* is non–positive and 0 otherwise.

whereZero(*a*[, *tol=0.*])
: returns a function which is 1 where *a* equals zero with tolerance *tol* and 0 otherwise.

whereNonZero(*a*[, *tol=0.*])
: returns a function which is 1 where *a* different from zero with tolerance *tol* and 0 otherwise.

3.1.7 `Operator` Class

The `Operator` class provides an abstract access to operators build within the `LinearPDE` class. `Operator` objects are created when a PDE is handed over to a PDE solver library and handled by the `LinearPDE` object defining the PDE. The user can gain access to the `Operator` of a `LinearPDE` object through the *getOperator* method.

class Operator()
: creates an empty `Operator` object.

isEmpty(*fileName*)
: returns `True` is the object is empty. Otherwise `True` is returned.

setValue(*value*)
: resets all entries in the object representation to *value*

solves(*rhs*)
: solves the operator equation with right hand side *rhs*

of(*u*)
: applies the operator to the `Data` object *u*

saveMM(*fileName*)
: saves the object to a matrix market format file of name *fileName*, see maths.nist.gov/MatrixMarket.

CHAPTER

FOUR

The Module `esys.escript.linearPDEs`

4.1 Linear Partial Differential Equations

The `LinearPDE` class is used to define a general linear, steady, second order PDE for an unknown function u on a given Ω defined through a `Domain` object. In the following Γ denotes the boundary of the domain Ω. n denotes the outer normal field on Γ.

For a single PDE with a solution with a single component the linear PDE is defined in the following form:

$$-(A_{jl}u_{,l})_{,j} - (B_j u)_{,j} + C_l u_{,l} + Du = -X_{j,j} + Y \ . \tag{4.1}$$

u, j denotes the derivative of u with respect to the j-th spatial direction. Einstein's summation convention, ie. summation over indexes appearing twice in a term of a sum is performed, is used. The coefficients A, B, C, D, X and Y have to be specified through `Data` objects in the general `FunctionSpace` on the PDE or objects that can be converted into such `Data` objects. A is a rank-2 `Data` object, B, C and X are rank-1 `Data` object and D and Y are scalar. The following natural boundary conditions are considered on Γ:

$$n_j(A_{jl}u_{,l} + B_j u) + du = n_j X_j + y \ . \tag{4.2}$$

Notice that the coefficients A, B and X are defined in the PDE. The coefficients d and y are each a scalar `Data` object in the boundary `FunctionSpace`. Constraints for the solution prescribing the value of the solution at certain locations in the domain. They have the form

$$u = r \text{ where } q > 0 \tag{4.3}$$

r and q are each scalar `Data` object where q is the characteristic function defining where the constraint is applied. The constraints defined by Equation (4.3) override any other condition set by Equation (4.1) or Equation (4.2).

For a system of PDEs and a solution with several components the PDE has the form

$$-(A_{ijkl}u_{k,l})_{,j} - (B_{ijk}u_k)_{,j} + C_{ikl}u_{k,l} + D_{ik}u_k = -X_{ij,j} + Y_i \ . \tag{4.4}$$

A is a rank-4 `Data` object, B and C are each a rank-3 `Data` object, D and X are each a rank-2 `Data` object and Y is a rank-1 `Data` object. The natural boundary conditions take the form:

$$n_j(A_{ijkl}u_{k,l} + B_{ijk}u_k) + d_{ik}u_k = n_j X_{ij} + y_i \ . \tag{4.5}$$

The coefficient d is a rank-2 `Data` object and y is a rank-1 `Data` object both in the boundary `FunctionSpace`. Constraints take the form

$$u_i = r_i \text{ where } q_i > 0 \tag{4.6}$$

r and q are each rank-1 `Data` object. Notice that not necessarily all components must have a constraint at all locations.

`LinearPDE` also supports solution discontinuities over contact region $\Gamma^{contact}$ in the domain Ω. To specify the conditions across the discontinuity we are using the generalised flux J which is in the case of a systems of PDEs and several components of the solution defined as

$$J_{ij} = A_{ijkl}u_{k,l} + B_{ijk}u_k - X_{ij} \tag{4.7}$$

For the case of single solution component and single PDE J is defined

$$J_j = A_{jl} u_{,l} + B_j u_k - X_j \tag{4.8}$$

In the context of discontinuities n denotes the normal on the discontinuity pointing from side 0 towards side 1. For a system of PDEs the contact condition takes the form

$$n_j J^0_{ij} = n_j J^1_{ij} = y^{contact}_i - d^{contact}_{ik} [u]_k \ . \tag{4.9}$$

where J^0 and J^1 are the fluxes on side 0 and side 1 of the discontinuity $\Gamma^{contact}$, respectively. $[u]$, which is the difference of the solution at side 1 and at side 0, denotes the jump of u across $\Gamma^{contact}$. The coefficient $d^{contact}$ is a rank-2 `Data` object and $y^{contact}$ is a rank-1 `Data` object both in the contact `FunctionSpace` on side 0 or contact `FunctionSpace` on side 1. In case of a single PDE and a single component solution the contact condition takes the form

$$n_j J^0_j = n_j J^1_j = y^{contact} - d^{contact} [u] \tag{4.10}$$

In this case the the coefficient $d^{contact}$ and $y^{contact}$ are each scalar `Data` object both in the contact `FunctionSpace` on side 0 or contact `FunctionSpace` on side 1.

The PDE is symmetrical if

$$A_{jl} = A_{lj} \text{ and } B_j = C_j \tag{4.11}$$

The system of PDEs is symmetrical if

$$A_{ijkl} = A_{klij} \tag{4.12}$$
$$B_{ijk} = C_{kij} \tag{4.13}$$
$$D_{ik} = D_{ki} \tag{4.14}$$
$$d_{ik} = d_{ki} \tag{4.15}$$
$$d^{contact}_{ik} = d^{contact}_{ki} \tag{4.16}$$

Note that in contrast with the scalar case Equation (4.11) now the coefficients D, d abd $d^{contact}$ have to be inspected.

4.1.1 Classes

The module `esys.escript.linearPDEs` provides an interface to define and solve linear partial differential equations within `esys.escript`. The module `esys.escript.linearPDEs` does not provide any solver capabilities in itself but hands the PDE over to the PDE solver library defined through the `Domain` of the PDE. The general interface is provided through the `LinearPDE` class. The `AdvectivePDE` which is derived from the `LinearPDE` class provides an interface to a PDE dominated by its advective terms. The `Poisson` class which is also derived form the `LinearPDE` class should be used to define the Poisson equation .

4.1.2 `LinearPDE` class

This is the general class to define a linear PDE in `esys.escript`. We list a selection of the most important methods of the class. For a complete list, see the reference at http://shake200.esscc.uq.edu.au/esys/esys13/release/epydoc/index.html.

class `LinearPDE`(*domain,numEquations=0,numSolutions=0*)
opens a linear, steady, second order PDE on the `Domain` *domain*. *numEquations* and *numSolutions* gives the number of equations and the number of solution components. If *numEquations* and *numSolutions* is non-positive, the number of equations and the number solutions, respectively, stay undefined until a coefficient is defined.

`LinearPDE` methods

`setValue`([*A*][, *B*], [, *C*][, *D*] [, *X*][, *Y*] [, *d*][, *y*] [, *d_contact*][, *y_contact*] [, *q*][, *r*])
assigns new values to coefficients. By default all values are assumed to be zero[1] If the new coefficient value is not a `Data` object, it is converted into a `Data` object in the appropriate `FunctionSpace`.

[1]In fact it is assumed they are not present by assigning the value `escript.Data()`. The can by used by the solver library to reduce computational costs.

getCoefficient(*name*)
: return the value assigned to coefficient *name*. If *name* is not a valid name an exception is raised.

getShapeOfCoefficient(*name*)
: returns the shape of coefficient *name* even if no value has been assigned to it.

getFunctionSpaceForCoefficient(*name*)
: returns the `FunctionSpace` of coefficient *name* even if no value has been assigned to it.

setDebugOn()
: switches on debug mode.

setDebugOff()
: switches off debug mode.

isUsingLumping()
: returns `True` if `LinearPDE.LUMPING` is set as the solver for the system of linear equations. Otherwise `False` is returned.

setSolverMethod([*solver=LinearPDE.DEFAULT*][*, preconditioner=LinearPDE.DEFAULT*])
: sets the solver method and preconditioner to be used. It should be noted that a PDE solver library may not know the specified solver method but may choose a similar method and preconditioner.

getSolverMethodName()
: returns the name of the solver method and preconditioner which is in use.

getSolverMethod()
: returns the solver method and preconditioner which is in use.

setSolverPackage([*package=LinearPDE.DEFAULT*])
: sets the solver package to be used by PDE library to solve the linear systems of equations. The specified package may not be supported by the PDE solver library. In this case, depending on the PDE solver, the default solver is used or an exception is thrown. If *package* is not specified, the default package of the PDE solver library is used.

getSolverPackage()
: returns the linear solver package currently by the PDE solver library

setTolerance([*tol=1.e-8*])
: resets the tolerance for solution. The actually meaning of tolerance depends on the underlying PDE library. In most cases, the tolerance will only consider the error from solving the discrete problem but will not consider any discretization error.

setToleranceReductionFactor(*TOL*)
: lowers the tolerance by a factor of TOL.

getTolerance()
: returns the current tolerance of the solution

getDomain()
: returns the `Domain` of the PDE.

getDim()
: returns the spatial dimension of the PDE.

getNumEquations()
: returns the number of equations.

getNumSolutions()
: returns the number of components of the solution.

checkSymmetry(*verbose*=`False`)
: returns `True` if the PDE is symmetric and `False` otherwise. The method is very computationally expensive and should only be called for testing purposes. The symmetry flag is not altered. If *verbose*=`True` information about where symmetry is violated are printed.

getFlux(*u*)
: returns the flux J_{ij} for given solution *u* defined by Equation (4.7) and Equation (4.8), respectively.

isSymmetric()
returns True if the PDE has been indicated to be symmetric. Otherwise False is returned.

setSymmetryOn()
indicates that the PDE is symmetric.

setSymmetryOff()
indicates that the PDE is not symmetric.

setReducedOrderOn()
switches on the reduction of polynomial order for the solution and equation evaluation even if a quadratic or higher interpolation order is defined in the Domain. This feature may not be supported by all PDE libraries.

setReducedOrderOff()
switches off the reduction of polynomial order for the solution and equation evaluation.

getOperator()
returns the Operator of the PDE.

getRightHandSide()
returns the right hand side of the PDE as a Data object. If *ignoreConstraint*=True, then the constraints are not considered when building up the right hand side.

getSystem()
returns the Operator and right hand side of the PDE.

getSolution([*verbose=False*] [, *reordering=LinearPDE.NO_REORDERING*] [, *iter_max=1000*] [, *drop_tolerance=0.01*] [, *drop_storage=1.20*] [, *truncation=-1*] [, *restart=-1*])
returns (an approximation of) the solution of the PDE. If verbose=True , then some information is printed during the solution process. *reordering* selects a reordering methods that is applied before or during the solution process (=LinearPDE.NO_REORDERING, LinearPDE.MINIMUM_FILL_IN , LinearPDE.NESTED_DISSECTION). *iter_max* specifies the maximum number of iteration steps that are allowed to reach the specified tolerance. *drop_tolerance* specifies a relative tolerance for small elements to be dropped when building a preconditioner (eg. in LinearPDE.ILUT). *drop_storage* limits the extra storage allowed when building a preconditioner (eg. in LinearPDE.ILUT). The extra storage is given relative to the size of the stiffness matrix, eg. *drop_storage=1.2* will allow the preconditioner to use the 1.2 fold storage space than used for the stiffness matrix. *truncation* defines the truncation.

LinearPDE symbols/members

DEFAULT
default method, preconditioner or package to be used to solve the PDE. An appropriate method should be chosen by the used PDE solver library.

SCSL
the SCSL library by SGI, Reference [**?**][2]

MKL
the MKL library by Intel, Reference [2][3].

UMFPACK
the UMFPACK, Reference [1]. Remark: UMFPACK is not parallelized.

PASO
the solver library of esys.finley, see Section 8.

ITERATIVE
the default iterative method and preconditioner. The actually used method depends on the PDE solver library and the solver package been chosen. Typically, LinearPDE.PCG is used for symmetric PDEs and LinearPDE.BICGSTAB otherwise, both with LinearPDE.JACOBI preconditioner.

DIRECT
the default direct linear solver.

[2]The SCSL library will only be available on SGI systems
[3]The MKL library will only be available when the Intel compilation environment is used.

CHOLEVSKY
direct solver based on Cholevsky factorization (or similar), see Reference [12]. The solver will require a symmetric PDE.

PCG
preconditioned conjugate gradient method, see Reference [17]. The solver will require a symmetric PDE.

TFQMR
transpose-free quasi-minimal residual method, see Reference [17].

GMRES
the GMRES method, see Reference [17]. Truncation and restart are controlled by the parameters *truncation* and *restart* of `getSolution`.

MINRES
minimal residual method method,

LUMPING
uses lumping to solve the system of linear equations . This solver technique condenses the stiffness matrix to a diagonal matrix so the solution of the linear systems becomes very cheap. It can be used when only D is present but in any case has to applied with care. The difference in the solutions with and without lumping can be significant but is expected to converge to zero when the mesh gets finer. Lumping does not use the linear system solver library.

PRES20
the GMRES method with truncation after five residuals and restart after 20 steps, see Reference [17].

CGS
conjugate gradient squared method, see Reference [17].

BICGSTAB
stabilized bi-conjugate gradients methods, see Reference [17].

SSOR
symmetric successive over-relaxation method, see Reference [17]. Typically used as preconditioner but some linear solver libraries support this as a solver.

ILU0
the incomplete LU factorization preconditioner with no fill-in, see Reference [12].

ILUT
the incomplete LU factorization preconditioner with fill-in, see Reference [12]. During the LU-factorization element with relative size less then *drop_tolerance* are dropped. Moreover, the size of the LU-factorization is restricted to the *drop_storage*-fold of the stiffness matrix. *drop_tolerance* and *drop_storage* are both set in the `getSolution` call.

JACOBI
the Jacobi preconditioner, see Reference [12].

AMG
the algebraic–multi grid method, see Reference [13]. This method can be used as linear solver method but is more robust when used in a preconditioner.

GS
the symmetric Gauss-Seidel preconditioner, see Reference [12].

RILU
recursive incomplete LU factorization preconditioner, see Reference [**?**]. This method is similar to `LinearPDE.ILUT` but uses smoothing between levels. During the LU-factorization element with relative size less then *drop_tolerance* are dropped. Moreover, the size of the LU-factorization is restricted to the *drop_storage*-fold of the stiffness matrix. *drop_tolerance* and *drop_storage* are both set in the `getSolution` call.

NO_REORDERING
no ordering is used during factorization.

MINIMUM_FILL_IN

applies reordering before factorization using a fill-in minimization strategy. You have to check with the particular solver library or linear solver package if this is supported. In any case, it is advisable to apply reordering on the mesh to minimize fill-in.

NESTED_DISSECTION
applies reordering before factorization using a nested dissection strategy. You have to check with the particular solver library or linear solver package if this is supported. In any case, it is advisable to apply reordering on the mesh to minimize fill-in.

4.1.3 The `Poisson` Class

The `Poisson` class provides an easy way to define and solve the Poisson equation

$$-u_{,ii} = f \; . \tag{4.17}$$

with homogeneous boundary conditions

$$n_i u_{,i} = 0 \tag{4.18}$$

and homogeneous constraints

$$u = 0 \text{ where } q > 0 \tag{4.19}$$

f has to be a scalar `Data` object in the general `FunctionSpace` and q must be a scalar `Data` object in the solution `FunctionSpace`.

class `Poisson`(*domain*)
opens a Poisson equation on the `Domain` domain. `Poisson` is derived from `LinearPDE`.

`setValue`(*f=escript.Data(),q=escript.Data()*)
assigns new values to f and q.

4.1.4 The `Helmholtz` Class

The `Helmholtz` class defines the Helmholtz problem

$$\omega \; u - (k \; u_{,j})_{,j} = f \tag{4.20}$$

with natural boundary conditions

$$k \; u_{,j} n_{,j} = g - \alpha \; u \tag{4.21}$$

and constraints:

$$u = r \text{ where } q > 0 \tag{4.22}$$

ω, k, f have to be a scalar `Data` object in the general `FunctionSpace`, g and α must be a scalar `Data` object in the boundary `FunctionSpace`, and q and r must be a scalar `Data` object in the solution `FunctionSpace` or must be mapped or interpolated into the particular `FunctionSpace`.

class `Helmholtz`(*domain*)
opens a Helmholtz equation on the `Domain` domain. `Helmholtz` is derived from `LinearPDE`.

`setValue`([*omega*] [, *k*] [, *f*] [, *alpha*] [, *g*] [, *r*] [, *q*])
assigns new values to *omega*, *k*, *f*, *alpha*, *g*, *r*, *q*. By default all values are set to be zero.

4.1.5 The `Lame` Class

The `Lame` class defines a Lame equation problem:

$$-\mu(u_{i,j} + u_{j,i}) + \lambda u_{k,k})_j = F_i - \sigma_{ij,j} \tag{4.23}$$

with natural boundary conditions:

$$n_j(\mu \; (u_{i,j} + u_{j,i}) + \lambda * u_{k,k}) = f_i + n_j \sigma_{ij} \tag{4.24}$$

and constraint

$$u_i = r_i \text{ where } q_i > 0 \tag{4.25}$$

μ, λ have to be a scalar `Data` object in the general `FunctionSpace`, F has to be a vector `Data` object in the general `FunctionSpace`, σ has to be a tensor `Data` object in the general `FunctionSpace`, f must be a vector `Data` object in the boundary `FunctionSpace`, and q and r must be a vector `Data` object in the solution `FunctionSpace` or must be mapped or interpolated into the particular `FunctionSpace`.

class **`Lame`**`(`*domain*`)`

opens a Lame equation on the `Domain` domain. `Lame` is derived from `LinearPDE`.

`setValue``(` [*lame_lambda*] [, *lame_mu*] [, *F*] [, *sigma*] [, *f*] [, *r*] [, *q*]`)`

assigns new values to *lame_lambda*, *lame_mu*, *F*, *sigma*, *f*, *r* and *q* By default all values are set to be zero.

CHAPTER

FIVE

The Module `esys.pycad`

5.1 Introduction

`esys.pycad` provides a simple way to build a mesh for your finite element simulation. You begin by building what we call a *Design* using primitive geometric objects, and then to go on to build a mesh from the *Design*. The final step of generating the mesh from a *Design* uses freely available mesh generation software, such as *Gmsh*[**?**] .

A *Design* is built by defining points, which are used to specify the corners of geometric objects and the vertices of curves. Using points you construct more interesting objects such as lines, rectangles, and arcs. By adding many of these objects into what we call a *Design*, you can build meshes for arbitrarily complex 2-D and 3-D structures.

The example included below shows how to use *pycad* to create a 2-D mesh in the shape of a trapezoid with a cutout area.

```
from esys.pycad import *
from esys.pycad.gmsh import Design
from esys.finley import MakeDomain

# A trapezoid
p0=Point(0.0, 0.0, 0.0)
p1=Point(1.0, 0.0, 0.0)
p2=Point(1.0, 0.5, 0.0)
p3=Point(0.0, 1.0, 0.0)
l01=Line(p0, p1)
l12=Line(p1, p2)
l23=Line(p2, p3)
l30=Line(p3, p0)
c=CurveLoop(l01, l12, l23, l30)

# A small triangular cutout
x0=Point(0.1, 0.1, 0.0)
x1=Point(0.5, 0.1, 0.0)
x2=Point(0.5, 0.2, 0.0)
x01=Line(x0, x1)
x12=Line(x1, x2)
x20=Line(x2, x0)
cutout=CurveLoop(x01, x12, x20)

# Create the surface with cutout
s=PlaneSurface(c, holes=[cutout])

# Create a Design which can make the mesh
d=Design(dim=2, element_size=0.05)

# Add the trapezoid with cutout
d.addItems(s)

# Create the geometry, mesh and Escript domain
d.setScriptFileName("trapezoid.geo")
```

```
d.setMeshFileName("trapezoid.msh")
domain=MakeDomain(d, integrationOrder=-1, reducedIntegrationOrder=-1, optimizeLabeling=True)

# Create a file that can be read back in to python with mesh=ReadMesh(fileName)
domain.write("trapezoid.fly")
```

This example is included with the software in `pycad/examples/trapezoid.py`. If you have gmsh installed you can run the example and view the geometry and mesh with:

```
python trapezoid.py
gmsh trapezoid.geo
gmsh trapezoid.msh
```

A `CurveLoop` is used to connect several lines into a single curve. It is used in the example above to create the trapezoidal outline for the grid and also for the triangular cutout area. You can use any number of lines when creating a `CurveLoop`, but the end of one line must be identical to the start of the next.

Sometimes you might see us write `-c` where `c` is a `CurveLoop`. This is the reverse curve of the curve `c`. It is identical to the original except that its points are traversed in the opposite order. This may make it easier to connect two curves in a `CurveLoop`.

The example python script above calls both `d.setScriptFileName()` and `d.setMeshFileName()`. You need only call these if you wish to save the gmsh geometry and mesh files.

Note that the underlying mesh generation software will not accept all the geometries you can create with *pycad*. For example, *pycad* will happily allow you to create a 2-D *Design* that is a closed loop with some additional points or lines lying outside of the enclosed area, but gmsh will fail to create a mesh for it.

5.2 `esys.pycad` Classes

5.2.1 Primitives

Some of the most commonly-used objects in *pycad* are listed here. For a more complete list see the full API documentation.

class `Point`(*x1, x2, x3*)
Create a point with from coordinates.

class `Line`(*point1, point2*)
Create a line with between starting and ending points.

class `Curve`(*point1, point2, ...*)
Create a `Curve`, which is simply a list of points.

class `Spline`(*curve*)
Interpret a `Curve` using a spline.

class `BSpline`(*curve*)
Interpret a `Curve` using a b-spline.

class `BezierCurve`(*curve*)
Interpret a `Curve` using a Bezier curve.

class `CurveLoop`(*list*)
Create a closed `Curve` connecting the lines and/or points given in the `list`.

class `Arc`(*center_point, start_point, end_point*)
Create an arc by specifying a center for a circle and start and end points. An arc may subtend an angle of at most π radians.

class `PlaneSurface`(*loop,* [*holes=[list]*])
Create a surface for a 2-D mesh, which may have one or more holes.

class `RuledSurface`(*list*)
Create a surface that can be interpolated using transfinite interpolation.

class `SurfaceLoop`(*list*)
Create a loop of 2D primitives, which defines the shell of a volume.

class `Volume`(*loop*, [*holes=[list]*])
Create a volume for a 3-D mesh given a SurfaceLoop, which may have one or more holes.

class `PropertySet`(*list*)
Create a PropertySet given a list of 1-D, 2-D or 3-D items. See the section on Properties below for more information.

5.2.2 Transformations

Sometimes it's convenient to create an object and then make copies at different orientations and in different sizes. Transformations are used to move geometrical objects in the 3-dimensional space and to resize them.

class `Translation`([*b=[0,0,0]*])
defines a translation $x \rightarrow x + b$. *b* can be any object that can be converted into a `numarray` object of shape $(3,)$.

class `Rotatation`([*axis=[1,1,1]*, [*point = [0,0,0]*, [*angle=0*RAD*]]])
defines a rotation by *angle* around axis through point *point* and direction *axis*. *axis* and *point* can be any object that can be converted into a `numarray` object of shape $(3,)$. *axis* does not have to be normalized but must have positive length. The right hand rule [**?**] applies.

class `Dilation`([*factor=1.*, [*center=[0,0,0]*]])
defines a dilation by the expansion/contraction *factor* with *center* as the dilation center. *center* can be any object that can be converted into a `numarray` object of shape $(3,)$.

class `Reflection`([*normal=[1,1,1]*, [*offset=0*]])
defines a reflection on a plane defined in normal form $n^t x = d$ where n is the surface normal *normal* and d is the plane *offset*. *normal* can be any object that can be converted into a `numarray` object of shape $(3,)$. *normal* does not have to be normalized but must have positive length.

`DEG`
A constant to convert from degrees to an internal angle representation in radians. For instance use `90*DEG` for 90 degrees.

5.2.3 Properties

If you are building a larger geometry you may find it convenient to create it in smaller pieces and then assemble them into the whole. Property sets make this easy, and they allow you to name the smaller pieces for convenience.

Property sets are used to bundle a set of geometrical objects in a group. The group is identified by a name. Typically a property set is used to mark subregions with share the same material properties or to mark portions of the boundary. For efficiency, the `Design` class object assigns a integer to each of its property sets, a so-called tag . The appropriate tag is attached to the elements at generation time.

See the file `pycad/examples/quad.py` for an example using a *PropertySet*.

class `PropertySet`(*name,*items*)
defines a group geometrical objects which can be accessed through a *name* The objects in the tuple *items* mast all be `Manifold1D` , `Manifold2D` or `Manifold3D` objects.

`getManifoldClass`()
returns the manifold class `Manifold1D` , `Manifold2D` or `Manifold3D` expected from the items in the property set.

`getDim`()
returns the spatial dimension of the items in the property set.

`getName`()
returns the name of the set

`setName`(*name*)

sets the name. This name should be unique within a `Design`.

`addItem`(**items*)
: adds a tuple of items. They need to be objects of class `Manifold1D`, `Manifold2D` or `Manifold3D`.

`getItems`()
: returns the list of items

`clearItems`()
: clears the list of items

`getTag`()
: returns the tag used for this property set

5.3 Interface to the mesh generation software

The class and methods described here provide an interface to the mesh generation software, which is currently gmsh. This interface could be adopted to triangle or another mesh generation package if this is deemed to be desirable in the future.

class `Design`([*dim=3*, [*element_size=1.*, [*order=1*, [*keep_files=False*]]]])
: The `Design` describes the geometry defined by primitives to be meshed. The *dim* specifies the spatial dimension. The argument *element_size* defines the global element size which is multiplied by the local scale to set the element size at each `Point`. The argument *order* defines the element order to be used. If *keep_files* is set to `True` temporary files a kept otherwise they are removed when the instance of the class is deleted.

`setDim`([*dim=3*])
: sets the spatial dimension which needs to be 1, 2 or 3.

`getDim`()
: returns the spatial dimension.

`setElementOrder`([*order=1*])
: sets the element order which needs to be 1 or 2.

`getElementOrder`()
: returns the element order.

`setElementSize`([*element_size=1*])
: set the global element size. The local element size at a point is defined as the global element size multiplied by the local scale. The element size must be positive.

`getElementSize`()
: returns the global element size.

`DELAUNAY`
: the gmsh Delauny triangulator.

`TETGEN`
: the TetGen [**?**] triangulator.

`TETGEN`
: the NETGEN [**?**] triangulator.

`setKeepFilesOn`()
: work files are kept at the end of the generation.

`setKeepFilesOff`()
: work files are deleted at the end of the generation.

`keepFiles`()
: returns `True` if work files are kept. Otherwise `False` is returned.

`setScriptFileName`([*name=None*])
: set the filename for the gmsh input script. if no name is given a name with extension ”geo” is generated.

getScriptFileName()
returns the name of the file for the gmsh script.

setMeshFileName([*name=None*])
sets the name for the gmsh mesh file. if no name is given a name with extension ”msh” is generated.

getMeshFileName()
returns the name of the file for the gmsh msh

addItems(**items*)
adds the tuple of varitems. An item can be any primitive or a `PropertySet`. **Warning:** If a `PropertySet` is added as an item added object that are not part of a `PropertySet` are not considered in the messing.

getItems()
returns a list of the items

clearItems()
resets the items in design

getMeshHandler()
returns a handle to the mesh. The call of this method generates the mesh from the geometry and returns a mechanism to access the mesh data. In the current implementation this method returns a file name for a gmsh file containing the mesh data.

getScriptString()
returns the gmsh script to generate the mesh as a string.

getCommandString()
returns the gmsh command used to generate the mesh as string.

setOptions([*algorithm=None*, [*optimize_quality=True*,[*smoothing=1*]]])
sets options for the mesh generator. *algorithm* sets the algorithm to be used. The algorithm needs to be *Design.DELAUNAY Design.TETGEN* or *Design.NETGEN*. By default *Design.DELAUNAY* is used. *optimize_quality*=`True` invokes an optimization of the mesh quality. *smoothing* sets the number of smoothing steps to be applied to the mesh.

getTagMap()
returns a `TagMap` to map the name `PropertySet` in the class to tag numbers generated by gmsh.

CHAPTER

SIX

The Module `esys.pyvisi`

6.1 Introduction

`esys.pyvisi` is a Python module that is used to generate 2D and 3D visualizations for escript and its PDE solver finley. The module provides an easy to use interface to the *VTK* library (http://www.vtk.org/) to render (generate) surface maps and contours for scalar fields, arrows and streamlines for vector fields, and ellipsoids for tensor fields. There are three approaches for rendering an object. (1) Online - object is rendered on-screen with interaction capability (i.e. zoom and rotate), (2) Offline - object is rendered off-screen (no pop-up window) and (3) Display - object is rendered on-screen but with no interaction capability (on-the-fly animation). All three approaches have the option to save the rendered object as an image (e.g. jpeg) and subsequently converting a series of images into a movie (mpeg).

The following outlines the general steps to use Pyvisi:

1. Create a `Scene` instance - a window in which objects will be rendered on.
2. Create a data input instance (i.e. `DataCollector` or `ImageReader`) - reads the source data for visualization.
3. Create a data visualization object (i.e. `Map`, `Velocity`, `Ellipsoid`, `Contour`, `Carpet`, `StreamLine`, etc.) - creates a visual representation of the source data.
4. Create a `Camera` or `Light` instance - controls the viewing angle and lighting effects.
5. Render the object - using either the Online, Offline or Display approach.
6. Generate movie - converts a series of images into a movie. (optional)

$$scene \rightarrow data\ input \rightarrow data\ visualization \rightarrow camera\,/\,light \rightarrow render \rightarrow movie$$

6.2 `esys.pyvisi` Classes

The following subsections give a brief overview of the important classes and some of their corresponding methods. Please refer to http://shake200.esscc.uq.edu.au/esys/esys13/release/epydoc/index.html for full details.

6.2.1 Scene Classes

This section details the instances used to setup the viewing environment.

`Scene` class

class `Scene`(*renderer = Renderer.ONLINE, num_viewport = 1, x_size = 1152, y_size = 864* **)**

A scene is a window in which objects are to be rendered on. Only one scene needs to be created. However, a scene may be divided into four smaller windows called viewports (if needed). Each viewport in turn can render a different object.

The following are some of the methods available:

`setBackground`(*color*)
: Set the background color of the scene.

`render`(*image_name = None*)
: Render the object using either the Online, Offline or Display mode.

`Camera` class

class `Camera`(*scene, viewport = Viewport.SOUTH_WEST*)
: A camera controls the display angle of the rendered object and one is usually created for a `Scene`. However, if a `Scene` has four viewports, then a separate camera may be created for each viewport.

The following are some of the methods available:

`setFocalPoint`(*position*)
: Set the focal point of the camera.

`setPosition`(*position*)
: Set the position of the camera.

`azimuth`(*angle*)
: Rotate the camera to the left and right. The angle parameter is in degrees.

`elevation`(*angle*)
: Rotate the camera up and down (angle must be between -90 and 90).

`backView`()
: Rotate the camera to view the back of the rendered object.

`topView`()
: Rotate the camera to view the top of the rendered object.

`bottomView`()
: Rotate the camera to view the bottom of the rendered object.

`leftView`()
: Rotate the camera to view the left side of the rendered object.

`rightView`()
: Rotate the camera to view the right side of the rendered object.

`isometricView`()
: Rotate the camera to view an isometric projection of the rendered object.

`dolly`(*distance*)
: Move the camera towards (greater than 1) the rendered object. However, it is not possible to move the camera away from the rendered object with this method.

`Light` class

class `Light`(*scene, viewport = Viewport.SOUTH_WEST*)
: A light controls the lighting effect for the rendered object and is set up in a similar way to `Camera`.

The following are some of the methods available:

`setColor`(*color*)
: Set the light color.

`setFocalPoint`(*position*)
: Set the focal point of the light.

`setPosition`(*position*)
: Set the position of the light.

`setAngle`(*elevation = 0, azimuth = 0*)
An alternative to set the position and focal point of the light by using elevation and azimuth.

6.2.2 Input Classes

This subsection details the instances used to read and load the source data for visualization.

`DataCollector` class

class `DataCollector`(*source = Source.XML*)
A data collector is used to read data either from an XML file (using `setFileName()`) or from an escript object directly (using `setData()`). Writing XML files is expensive but has the advantage that the results can be analyzed easily after the simulation has completed.

The following are some of the methods available:

`setFileName`(*file_name*)
Set the XML file name to read.

`setData`(***args*)
Create data using the <name>=<data>pairing. The method assumes that the data is given in the appropriate format.

`setActiveScalar`(*scalar*)
Specify the scalar field to load.

`setActiveVector`(*vector*)
Specify the vector field to load.

`setActiveTensor`(*tensor*)
Specify the tensor field to load.

`ImageReader` class

class `ImageReader`(*format*)
An image reader is used to read data from an image in a variety of formats.

The following is one of the methods available:

`setImageName`(*image_name*)
Set the filename of the image to be loaded.

`Text2D` class

class `Text2D`(*scene, text, viewport = Viewport.SOUTH_WEST*)
This class is used to insert two-dimensional text for annotations (e.g. titles, authors and labels).

The following are some of the methods available:

`setFontSize`(*size*)
Set the 2D text size.

`boldOn`( )
Use bold font style for the text.

`setColor`(*color*)
Set the color of the 2D text.

Including methods from `Actor2D`.

6.2.3 Data Visualization Classes

This subsection details the instances used to process and manipulate the source data. The typical usage of some of the classes is also shown. See Section 6.5 for sample images generated with these classes.

One point to note is that the source can either be point or cell data. If the source is cell data, a conversion to point data may or may not be required, in order for the object to be rendered correctly. If a conversion is needed, the 'cell_to_point' flag (see below) must be set to 'True', otherwise to 'False' (which is the default). On occasions, an inaccurate object may be rendered from cell data even after conversion.

Map class

class `Map`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

Class that shows a scalar field on a domain surface. The domain surface can either be color or gray-scale, depending on the lookup table used.

The following are some of the methods available:
Methods from `Actor3D` and `DataSetMapper`.

A typical usage of `Map` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, Map, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 800
Y_SIZE = 800

SCALAR_FIELD_POINT_DATA = "temperature"
SCALAR_FIELD_CELL_DATA = "temperature_cell"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "map.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene with four viewports.
s = Scene(renderer = JPG_RENDERER, num_viewport = 4, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
dc1.setActiveScalar(scalar = SCALAR_FIELD_POINT_DATA)

# Create a  Map for the first viewport.
m1 = Map(scene = s, data_collector = dc1, viewport = Viewport.SOUTH_WEST,
        lut = Lut.COLOR, cell_to_point = False, outline = True)
m1.setRepresentationToWireframe()

# Create a Camera for the first viewport
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
c1.isometricView()

# Create a second DataCollector reading from the same XML file but specifying
# a different scalar field.
dc2 = DataCollector(source = Source.XML)
dc2.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
```

```
dc2.setActiveScalar(scalar = SCALAR_FIELD_CELL_DATA)

# Create a Map for the third viewport.
m2 = Map(scene = s, data_collector = dc2, viewport = Viewport.NORTH_EAST,
        lut = Lut.COLOR, cell_to_point = True, outline = True)

# Create a Camera for the third viewport
c2 = Camera(scene = s, viewport = Viewport.NORTH_EAST)

# Render the object.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME))
```

`MapOnPlaneCut` class

class `MapOnPlaneCut`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `Map`, except that the result is a slice of the scalar field produced by cutting the map with a plane. The plane can be translated and rotated to its desired position.

The following are some of the methods available:
Methods from `Actor3D`, `Transform` and `DataSetMapper`.

`MapOnPlaneClip` class

class `MapOnPlaneClip`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneCut`, except that the defined plane is used to clip the scalar field.

The following are some of the methods available:
Methods from `Actor3D`, `Transform`, `Clipper` and `DataSetMapper`.

`MapOnScalarClip` class

class `MapOnScalarClip`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `Map`, except that it only shows parts of the scalar field matching a scalar value.

The following are some of the methods available:
Methods from `Actor3D`, `Clipper` and `DataSetMapper`.

`MapOnScalarClipWithRotation` class

class `MapOnScalarClipWithRotation`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False*)

This class works in a similar way to `Map` except that it shows a 2D scalar field clipped using a scalar value and subsequently rotated around the z-axis to create a 3D looking effect. This class should only be used with 2D data sets and NOT 3D.

The following are some of the methods available:
Methods from `Actor3D`, `Clipper`, `Rotation` and `DataSetMapper`.

`Velocity` class

class `Velocity`(*scene, data_collector, arrow = Arrow.TWO_D, color_mode = ColorMode.VECTOR, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class is used to display a vector field using arrows. The arrows can either be color or gray-scale, depending on the lookup table used. If the arrows are colored, there are two possible coloring modes, either using vector data or scalar data. Similarly, there are two possible types of arrows, either two-dimensional or three-dimensional.

The following are some of the methods available:
Methods from `Actor3D`, `Glyph3D`, `MaskPoints` and `DataSetMapper`.

`VelocityOnPlaneCut` class

class **`VelocityOnPlaneCut`**(*scene, data_collector, arrow = Arrow.TWO_D, color_mode = ColorMode.VECTOR, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneCut`, except that it shows a vector field using arrows cut using a plane.

The following are some of the methods available:
Methods from `Actor3D`, `Glyph3D`, `Transform`, `MaskPoints` and `DataSetMapper`.

A typical usage of `VelocityOnPlaneCut` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules
from esys.pyvisi import Scene, DataCollector, VelocityOnPlaneCut, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400

VECTOR_FIELD_CELL_DATA = "velocity"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "velocity.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
dc1.setActiveVector(vector = VECTOR_FIELD_CELL_DATA)

# Create VelocityOnPlaneCut.
vopc1 = VelocityOnPlaneCut(scene = s, data_collector = dc1,
        viewport = Viewport.SOUTH_WEST, color_mode = ColorMode.VECTOR,
        arrow = Arrow.THREE_D, lut = Lut.COLOR, cell_to_point = False,
        outline = True)
vopc1.setScaleFactor(scale_factor = 0.5)
vopc1.setPlaneToXY(offset = 0.5)
vopc1.setRatio(2)
vopc1.randomOn()

# Create a Camera.
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
c1.isometricView()
c1.elevation(angle = -20)

# Render the object.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME))
```

`VelocityOnPlaneClip` class

class `VelocityOnPlaneClip`(*scene, data_collector, arrow = Arrow.TWO_D, color_mode = ColorMode.VECTOR, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, online = True*)

This class works in a similar way to `MapOnPlaneClip`, except that it shows a vector field using arrows clipped using a plane.

The following are some of the methods available:
Methods from `Actor3D`, `Glyph3D`, `Transform`, `Clipper`, `MaskPoints` and `DataSetMapper`.

`Ellipsoid` class

class `Ellipsoid`(*scene, data_collector, viewport = Viewport = SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

Class that shows a tensor field using ellipsoids. The ellipsoids can either be color or gray-scale, depending on the lookup table used.

The following are some of the methods available:
Methods from `Actor3D`, `Sphere`, `TensorGlyph`, `MaskPoints` and `DataSetMapper`.

`EllipsoidOnPlaneCut` class

class `EllipsoidOnPlaneCut`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneCut`, except that it shows a tensor field using ellipsoids cut using a plane.

The following are some of the methods available:
Methods from `Actor3D`, `Sphere`, `TensorGlyph`, `Transform`, `MaskPoints` and `DataSetMapper`.

`EllipsoidOnPlaneClip` class

class `EllipsoidOnPlaneClip`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneClip`, except that it shows a tensor field using ellipsoids clipped using a plane.

The following are some of the methods available:
Methods from `Actor3D`, `Sphere`, `TensorGlyph`, `Transform`, `Clipper`, `MaskPoints` and `DataSetMapper`.

A typical usage of `EllipsoidOnPlaneClip` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules
from esys.pyvisi import Scene, DataCollector, EllipsoidOnPlaneClip, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400

TENSOR_FIELD_CELL_DATA = "stress_cell"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "ellipsoid.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG
```

```
# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
dc1.setActiveTensor(tensor = TENSOR_FIELD_CELL_DATA)

# Create an EllipsoidOnPlaneClip.
eopc1 = EllipsoidOnPlaneClip(scene = s, data_collector = dc1,
        viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = True,
        outline = True)
eopc1.setPlaneToXY()
eopc1.setScaleFactor(scale_factor = 0.2)
eopc1.rotateX(angle = 10)

# Create a Camera.
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
c1.bottomView()
c1.azimuth(angle = -90)
c1.elevation(angle = 10)

# Render the object.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME))
```

`Contour` class

class `Contour`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

Class that shows a scalar field using contour surfaces. The contour surfaces can either be color or gray-scale, depending on the lookup table used. This class can also be used to generate isosurfaces.

The following are some of the methods available:
Methods from `Actor3D`, `ContourModule` and `DataSetMapper`.

A typical usage of `Contour` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules
from esys.pyvisi import Scene, DataCollector, Contour, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400

SCALAR_FIELD_POINT_DATA = "temperature"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "contour.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading a XML file.
```

```
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
dc1.setActiveScalar(scalar = SCALAR_FIELD_POINT_DATA)

# Create three contours.
ctr1 = Contour(scene = s, data_collector = dc1, viewport = Viewport.SOUTH_WEST,
        lut = Lut.COLOR, cell_to_point = False, outline = True)
ctr1.generateContours(contours = 3)

# Create a Camera.
cam1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
cam1.elevation(angle = -40)

# Render the object.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME))
```

`ContourOnPlaneCut` class

class `ContourOnPlaneCut`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneCut`, except that it shows a scalar field using contour surfaces cut using a plane.

The following are some of the methods available:
Methods from `Actor3D`, `ContourModule`, `Transform` and `DataSetMapper`.

`ContourOnPlaneClip` class

class `ContourOnPlaneClip`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneClip`, except that it shows a scalar field using contour surfaces clipped using a plane.

The following are some of the methods available:
Methods from `Actor3D`, `ContourModule`, `Transform`, `Clipper` and `DataSetMapper`.

`StreamLine` class

class `StreamLine`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, color_mode = ColorMode.VECTOR, lut = Lut.COLOR, cell_to_point = False, outline = True*)

Class that shows the direction of particles of a vector field using streamlines. The streamlines can either be color or gray-scale, depending on the lookup table used. If the streamlines are colored, there are two possible coloring modes, either using vector data or scalar data.

The following are some of the methods available:
Methods from `Actor3D`, `PointSource`, `StreamLineModule`, `Tube` and `DataSetMapper`.

A typical usage of `StreamLine` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, StreamLine, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
```

```
Y_SIZE = 400

VECTOR_FIELD_CELL_DATA = "temperature"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "streamline.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))

# Create streamlines.
sl1 = StreamLine(scene = s, data_collector = dc1,
        viewport = Viewport.SOUTH_WEST, color_mode = ColorMode.SCALAR,
        lut = Lut.COLOR, cell_to_point = False, outline = True)
sl1.setTubeRadius(radius = 0.02)
sl1.setTubeNumberOfSides(3)
sl1.setTubeRadiusToVaryByVector()
sl1.setPointSourceRadius(0.9)

# Create a Camera.
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
c1.isometricView()

# Render the object.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME))
```

`Carpet` class

class `Carpet`(*scene, data_collector, viewport = Viewport.Viewport.SOUTH_WEST, warp_mode = WarpMode.SCALAR, lut = Lut.COLOR, cell_to_point = False, outline = True*)

This class works in a similar way to `MapOnPlaneCut`, except that it shows a scalar field cut on a plane and deformed (warped) along the normal. The plane can either be color or gray-scale, depending on the lookup table used. Similarly, the plane can be deformed either using scalar data or vector data.

The following are some of the methods available:
Methods from `Actor3D`, `Warp`, `Transform` and `DataSetMapper`.

A typical usage of `Carpet` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, Carpet, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400

SCALAR_FIELD_CELL_DATA = "temperature_cell"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "carpet.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG
```

```
# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
dc1.setActiveScalar(scalar = SCALAR_FIELD_CELL_DATA)

# Create a Carpet.
cpt1 = Carpet(scene = s, data_collector = dc1, viewport = Viewport.SOUTH_WEST,
        warp_mode = WarpMode.SCALAR, lut = Lut.COLOR, cell_to_point = True,
        outline = True)
cpt1.setPlaneToXY(0.2)
cpt1.setScaleFactor(1.9)

# Create a Camera.
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
c1.isometricView()

# Render the object.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME))
```

`Legend` class

class `Legend`(*scene, data_collector, viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, legend = LegendType.SCALAR*)
Class that shows a scalar field on a domain surface. The domain surface can either be color or gray-scale, depending on the lookup table used

The following are some of the methods available:
Methods from `Actor3D`, `ScalarBar` and `DataSetMapper`.

`Rectangle` class

class `Rectangle`(*scene, viewport = Viewport.SOUTH_WEST*)
Class that generates a rectangle box.

The following are some of the methods available:
Methods from `Actor3D`, `CubeSource` and `DataSetMapper`.

`Image` class

class `Image`(*scene, image_reader, viewport = Viewport.SOUTH_WEST*)
Class that displays an image which can be scaled (upwards and downwards) and has interaction capability. The image can also be translated and rotated along the X, Y and Z axes. One of the most common use of this feature is pasting an image on a surface map.

The following are some of the methods available:
Methods from `Actor3D`, `PlaneSource` and `Transform`.

A typical usage of `Image` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, Map, ImageReader, Image, Camera
from esys.pyvisi import GlobalPosition
from esys.pyvisi.constant import *
```

```
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400

SCALAR_FIELD_POINT_DATA = "temperature"
FILE_3D = "interior_3D.xml"
LOAD_IMAGE_NAME = "flinders.jpg"
SAVE_IMAGE_NAME = "image.jpg"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))

# Create a Map.
m1 = Map(scene = s, data_collector = dc1, viewport = Viewport.SOUTH_WEST,
        lut = Lut.COLOR, cell_to_point = False, outline = True)
m1.setOpacity(0.3)

# Create an ImageReader (in place of DataCollector).
ir = ImageReader(ImageFormat.JPG)
ir.setImageName(image_name =  os.path.join(PYVISI_EXAMPLE_MESHES_PATH, \
        LOAD_IMAGE_NAME))

# Create an Image.
i = Image(scene = s, image_reader = ir, viewport = Viewport.SOUTH_WEST)
i.setOpacity(opacity = 0.9)
i.translate(0,0,-1)
i.setPoint1(GlobalPosition(2,0,0))
i.setPoint2(GlobalPosition(0,2,0))

# Create a Camera.
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)

# Render the image.
s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, SAVE_IMAGE_NAME))
```

Logo class

class `Logo`(*scene, image_reader, viewport = Viewport.SOUTH_WEST*)

Class that displays a static image, in particular a logo (e.g. company symbol) and has NO interaction capability. The position and size of the logo can be specified.

The following are some of the methods available:
Methods from `ImageReslice` and `Actor2D`.

Movie class

class `Movie`(*parameter_file = "make_movie"*)

This class is used to create movies out of a series of images. The parameter specifies the name of a file that will contain the required information for the 'ppmtompeg' command which is used to generate the movie.

The following are some of the methods available:

imageRange(*input_directory, first_image, last_image*)
: Use this method to specify that the movie is to be generated from image files with filenames in a certain range (e.g. 'image000.jpg' to 'image050.jpg').

imageList(*input_directory, image_list*)
: Use this method to specify a list of arbitrary image filenames from which the movie is to be generated.

makeMovie(*movie*)
: Generate the movie with the specified filename.

A typical usage of `Movie` is shown below.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, Map, Camera, Velocity, Legend
from esys.pyvisi import Movie, LocalPosition
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 800
Y_SIZE = 800

SCALAR_FIELD_POINT_DATA = "temp"
FILE_2D = "tempvel-"
IMAGE_NAME = "movie"
JPG_RENDERER = Renderer.OFFLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from a XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setActiveScalar(scalar = SCALAR_FIELD_POINT_DATA)

# Create a Map.
m1 = Map(scene = s, data_collector = dc1,
        viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False,
        outline = True)

# Create a Camera.
cam1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)

# Create a movie.
mov = Movie()
lst = []

# Read in one file one after another and render the object.
for i in range(938, 949):
    dc1.setFileName(file_name =  os.path.join(PYVISI_EXAMPLE_MESHES_PATH, \
                FILE_2D + "%06d.vtu") % i)

    s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, \
            IMAGE_NAME + "%06d.jpg" % i))

    lst.append(IMAGE_NAME + "%06d.jpg" % i)

# Images (first and last inclusive) from which the movie is to be generated.
mov.imageRange(input_directory = PYVISI_EXAMPLE_IMAGES_PATH,
        first_image = IMAGE_NAME + "000938.jpg",
        last_image = IMAGE_NAME + "000948.jpg")

# Alternatively, a list of images can be specified.
#mov.imageList(input_directory = PYVISI_EXAMPLE_IMAGES_PATH, image_list = lst)

# Generate the movie.
mov.makeMovie(os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, "movie.mpg"))
```

6.2.4 Coordinate Classes

This subsection details the instances used to position rendered objects.

`LocalPosition` class

class `LocalPosition`(*x_coor, y_coor*)
    Class that defines a position (X and Y) in the local 2D coordinate system.

`GlobalPosition` class

class `GlobalPosition`(*x_coor, y_coor, z_coor*)
    Class that defines a position (X, Y and Z) in the global 3D coordinate system.

6.2.5 Supporting Classes

This subsection details the supporting classes and their corresponding methods inherited by the input (see Section 6.2.2) and data visualization classes (see Section 6.2.3).

`Actor3D` class

Class that defines a 3D actor.

The following are some of the methods available:

`setOpacity`(*opacity*)
    Set the opacity (transparency) of the 3D actor.

`setColor`(*color*)
    Set the color of the 3D actor.

`setRepresentationToWireframe`()
    Set the representation of the 3D actor to wireframe.

`Actor2D` class

Class that defines a 2D actor.

The following are some of the methods available:

`setPosition`(*position*)
    Set the position (XY) of the 2D actor. Default position is the lower left hand corner of the window / viewport.

`Clipper` class

Class that defines a clipper.

The following are some of the methods available:

setInsideOutOn()
: Clips one side of the rendered object.

setInsideOutOff()
: Clips the other side of the rendered object.

setClipValue(*value*)
: Set the scalar clip value (instead of using a plane) for the clipper.

`ContourModule` class

Class that defines the contour module.

The following are some of the methods available:

generateContours(*contours = None, lower_range = None, upper_range = None*)
: Generate the specified number of contours within the specified range. In order to generate a single isosurface, the 'lower_range' and 'upper_range' must be set to the same value.

`Glyph3D` class

Class that defines 3D glyphs.

The following are some of the methods available:

setScaleModeByVector()
: Set the 3D glyph to scale according to the vector data.

setScaleModeByScalar()
: Set the 3D glyph to scale according to the scalar data.

setScaleFactor(*scale_factor*)
: Set the 3D glyph scale factor.

`TensorGlyph` class

Class that defines tensor glyphs.

The following are some of the methods available:

setScaleFactor(*scale_factor*)
: Set the scale factor for the tensor glyph.

setMaxScaleFactor(*max_scale_factor*)
: Set the maximum allowable scale factor for the tensor glyph.

`PlaneSource` class

Class that defines a plane source. A plane source is defined by an origin and two other points, which form the axes (X and Y).

The following are some of the methods available:

setOrigin(*position*)
: Set the origin of the plane source.

`setPoint1`(*position*)
  Set the first point from the origin of the plane source.

`setPoint2`(*position*)
  Set the second point from the origin of the plane source.

`PointSource` class

Class that defines the source (location) to generate points. The points are generated within the radius of a sphere.

The following are some of the methods available:

`setPointSourceRadius`(*radius*)
  Set the radius of the sphere.

`setPointSourceCenter`(*center*)
  Set the center of the sphere.

`setPointSourceNumberOfPoints`(*points*)
  Set the number of points to generate within the sphere (the larger the number of points, the more streamlines are generated).

`Sphere` class

Class that defines a sphere.

The following are some of the methods available:

`setThetaResolution`(*resolution*)
  Set the theta resolution of the sphere.

`setPhiResolution`(*resolution*)
  Set the phi resolution of the sphere.

`StreamLineModule` class

Class that defines the streamline module.

The following are some of the methods available:

`setMaximumPropagationTime`(*time*)
  Set the maximum length of the streamline expressed in elapsed time.

`setIntegrationToBothDirections`()
  Set the integration to occur both sides: forward (where the streamline goes) and backward (where the streamline came from).

`Transform` class

Class that defines the orientation of planes.

The following are some of the methods available:

`translate`(*x_offset, y_offset, z_offset*)
  Translate the rendered object along the x, y and z-axes.

`rotateX`(*angle*)
  Rotate the plane around the x-axis.

`rotateY``(`*angle*`)`
: Rotate the plane around the y-axis.

`rotateZ``(`*angle*`)`
: Rotate the plane around the z-axis.

`setPlaneToXY``(`*offset = 0*`)`
: Set the plane orthogonal to the z-axis.

`setPlaneToYZ``(`*offset = 0*`)`
: Set the plane orthogonal to the x-axis.

`setPlaneToXZ``(`*offset = 0*`)`
: Set the plane orthogonal to the y-axis.

`Tube` class

Class that defines the tube wrapped around the streamlines.

The following are some of the methods available:

`setTubeRadius``(`*radius*`)`
: Set the radius of the tube.

`setTubeRadiusToVaryByVector``()`
: Set the radius of the tube to vary by vector data.

`setTubeRadiusToVaryByScalar``()`
: Set the radius of the tube to vary by scalar data.

`Warp` class

Class that defines the deformation of a scalar field.

The following are some of the methods available:

`setScaleFactor``(`*scale_factor*`)`
: Set the displacement scale factor.

`MaskPoints` class

Class that defines masking of points. This is useful to prevent the rendered object from being cluttered with arrows or ellipsoids.

The following are some of the methods available:

`setRatio``(`*ratio*`)`
: Mask every n'th point.

`randomOn``()`
: Enables randomization of the points selected for masking.

`ScalarBar` class

Class that defines a scalar bar.

The following are some of the methods available:

`setTitle`(*title*)
: Set the title of the scalar bar.

`setPosition`(*position*)
: Set the local position of the scalar bar.

`setOrientationToHorizontal`( )
: Set the orientation of the scalar bar to horizontal.

`setOrientationToVertical`( )
: Set the orientation of the scalar bar to vertical.

`setHeight`(*height*)
: Set the height of the scalar bar.

`setWidth`(*width*)
: Set the width of the scalar bar.

`setLabelColor`(*color*)
: Set the color of the scalar bar's label.

`setTitleColor`(*color*)
: Set the color of the scalar bar's title.

`ImageReslice` class

Class that defines an image reslice which is used to resize static (no interaction capability) images (i.e. logo).

The following are some of the methods available:

`setSize`(*size*)
: Set the size factor of the image. The value must be between 0 and 2. Size 1 (one) keeps the image in its original size (which is the default).

`DataSetMapper` class

Class that defines a data set mapper.

The following are some of the methods available:

`setScalarRange`(*lower_range, upper_range*)
: Set the minimum and maximum scalar range for the data set mapper. This method is called when the range has been specified by the user. Therefore, the scalar range read from the source will be ignored.

`CubeSource` class

Class that defines a cube source. The center of the cube source defines the point from which the cube is to be generated and the X, Y and Z lengths define the length of the cube from the center point. If X length is 3, then the X length to the left and right of the center point is 1.5 respectively.

The following are some of the methods available:

`setCenter`(*center*)
: Set the cube source center.

`setXLength`(*length*)
: Set the cube source length along the x-axis.

`setYLength`(*length*)
: Set the cube source length along the y-axis.

setZLength(*length*)
: Set the cube source length along the z-axis.

Rotation class

Class that sweeps 2D data around the z-axis to create a 3D looking effect.

The following are some of the methods available:

setResolution(*resolution*)
: Set the resolution of the sweep for the rotation, which controls the number of intermediate points.

setAngle(*angle*)
: Set the angle of rotation.

6.3 More Examples

This section provides examples for some common tasks.

6.3.1 Reading a Series of Files

The following script shows how to generate images from a time series using two data sources.

```python
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, Contour, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 300

SCALAR_FIELD_POINT_DATA_1 = "lava"
SCALAR_FIELD_POINT_DATA_2 = "talus"
FILE_2D = "phi_talus_lava."

IMAGE_NAME = "seriesofreads"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from an XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setActiveScalar(scalar = SCALAR_FIELD_POINT_DATA_1)

# Create a Contour.
mosc1 = Contour(scene = s, data_collector = dc1,
        viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False,
        outline = True)
mosc1.generateContours(0)

# Create a second DataCollector reading from the same XML file
# but specifying a different scalar field.
dc2 = DataCollector(source = Source.XML)
dc2.setActiveScalar(scalar = SCALAR_FIELD_POINT_DATA_2)

# Create a second Contour.
mosc2 = Contour(scene = s, data_collector = dc2,
        viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False,
        outline = True)
mosc2.generateContours(0)

# Create a Camera.
cam1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)

# Read in one file after another and render the object.
for i in range(99, 104):
    dc1.setFileName(file_name =  os.path.join(PYVISI_EXAMPLE_MESHES_PATH, \
                FILE_2D + "%04d.vtu") % i)
    dc2.setFileName(file_name =  os.path.join(PYVISI_EXAMPLE_MESHES_PATH, \
            FILE_2D + "%04d.vtu") % i)

    s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, \
            IMAGE_NAME + "%04d.jpg") % i)
```

6.3.2 Creating Slices of a Data Source

The following script shows how to save a series of images that slice the data at different points by gradually translating the cut plane.

```
"""
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.pyvisi import Scene, DataCollector, MapOnPlaneCut, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_MESHES_PATH = "data_meshes"
PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400

SCALAR_FIELD_POINT_DATA = "temperature"
FILE_3D = "interior_3D.xml"
IMAGE_NAME = "seriesofcuts"
JPG_RENDERER = Renderer.ONLINE_JPG

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, num_viewport = 1, x_size = X_SIZE,
        y_size = Y_SIZE)

# Create a DataCollector reading from an XML file.
dc1 = DataCollector(source = Source.XML)
dc1.setFileName(file_name = os.path.join(PYVISI_EXAMPLE_MESHES_PATH, FILE_3D))
dc1.setActiveScalar(scalar = SCALAR_FIELD_POINT_DATA)

# Create a MapOnPlaneCut.
mopc1 = MapOnPlaneCut(scene = s, data_collector = dc1,
        viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, cell_to_point = False,
        outline = True)
mopc1.setPlaneToYZ(offset = 0.1)
```

```
# Create a Camera.
c1 = Camera(scene = s, viewport = Viewport.SOUTH_WEST)
c1.isometricView()

# Render the object with multiple cuts using a series of translations.
for i in range(0, 5):
    s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, IMAGE_NAME +
                        "%02d.jpg") % i)
    mopc1.translate(0.6,0,0)
```

6.3.3 Reading Data Directly from escript Objects

The following script shows how to combine Pyvisi code with escript code to generate visualizations on the fly.

```
"""
Author: Lutz Gross, l.gross@uq.edu.au
Author: John Ngui, john.ngui@uq.edu.au
"""

# Import the necessary modules.
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Rectangle
from esys.pyvisi import Scene, DataCollector, Map, Camera
from esys.pyvisi.constant import *
import os

PYVISI_EXAMPLE_IMAGES_PATH = "data_sample_images"
X_SIZE = 400
Y_SIZE = 400
JPG_RENDERER = Renderer.ONLINE_JPG

#... set some parameters ...
xc = [0.02,0.002]
r = 0.001
qc = 50.e6
Tref = 0.
rhocp = 2.6e6
eta = 75.
kappa = 240.
tend = 5.
# initialize time, time step size and counter ...
t=0
h=0.1
i=0

# generate domain ...
mydomain = Rectangle(l0=0.05, l1=0.01, n0=250, n1=50)
# open PDE ...
mypde = LinearPDE(mydomain)
mypde.setSymmetryOn()
mypde.setValue(A=kappa*kronecker(mydomain), D=rhocp/h, d=eta, y=eta*Tref)
# set heat source: ...
x = mydomain.getX()
qH = qc*whereNegative(length(x-xc)-r)

# set initial temperature ....
T=Tref

# Create a Scene.
s = Scene(renderer = JPG_RENDERER, x_size = X_SIZE, y_size = Y_SIZE)
```

```
# Create a DataCollector reading directly from escript objects.
dc = DataCollector(source = Source.ESCRIPT)

# Create a Map.
m = Map(scene = s, data_collector = dc, \
        viewport = Viewport.SOUTH_WEST, lut = Lut.COLOR, \
        cell_to_point = False, outline = True)

# Create a Camera.
c = Camera(scene = s, viewport = Viewport.SOUTH_WEST)

# start iteration
while t < 0.4:
      i += 1
      t += h
      mypde.setValue(Y=qH+rhocp/h*T)
      T = mypde.getSolution()

      dc.setData(temp = T)

      # Render the object.
      s.render(image_name = os.path.join(PYVISI_EXAMPLE_IMAGES_PATH, \
              "diffusion%02d.jpg") % i)
```

6.4 Useful Keys

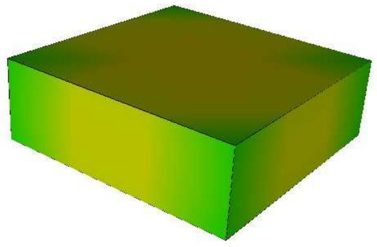
This section lists keyboard shortcuts available when interacting with rendered objects using the Online approach.

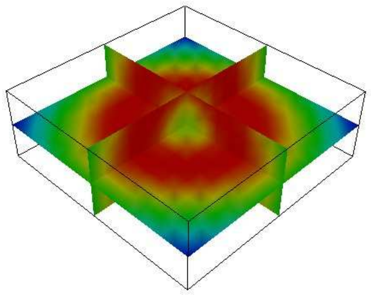
Key	**Description**
Keypress ’c’ / ’a’	Toggle between the camera (’c’) and object (’a’) mode. In camera mode, mouse events affect the camera position and focal point. In object mode, mouse events affect the rendered object’s element (i.e. cut surface map, clipped velocity field, streamline, etc) that is under the mouse pointer.
Mouse button 1	Rotate the camera around its focal point (if in camera mode) or rotate the rendered object’s element (if in object mode).
Mouse button 2	Pan the camera (if in camera mode) or translate the rendered object’s element (if in object mode).
Mouse button 3	Zoom the camera (if in camera mode) or scale the rendered object’s element (if in object mode).
Keypress 3	Toggle the render window in and out of stereo mode. By default, red-blue stereo pairs are created.
Keypress ’e’ / ’q’	Exit the application if only one file is to be read, or read and display the next file if multiple files are to be read.
Keypress ’s’	Modify the representation of the rendered object to surfaces.
Keypress ’w’	Modify the representation of the rendered object to wireframe.
Keypress ’r’	Reset the position of the rendered object to the center.

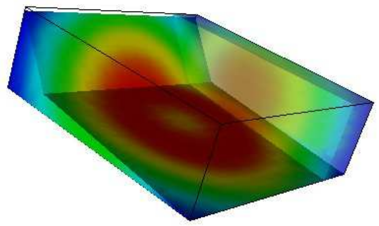
Table 6.1: Useful keys in Online render mode

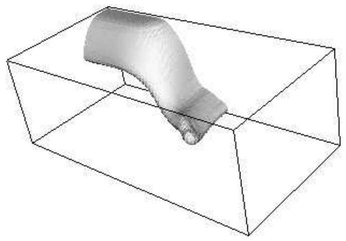
6.5 Sample Output

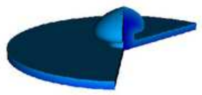
This section shows sample images produced with the various classes of Pyvisi. The source code to produce these images is included in the Pyvisi distribution.

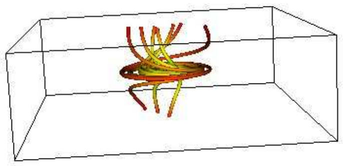

Map

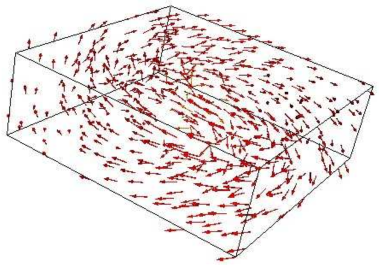

MapOnPlaneCut

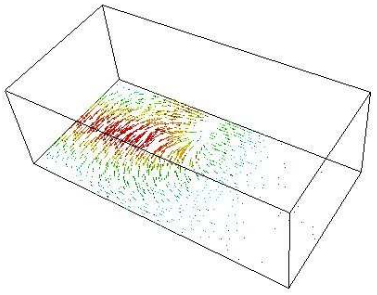

MapOnPlaneClip

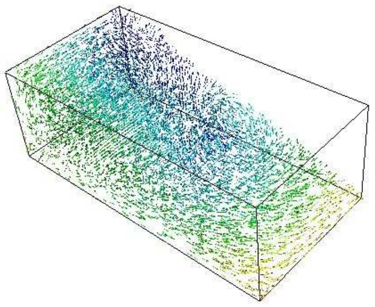

MapOnScalarClip

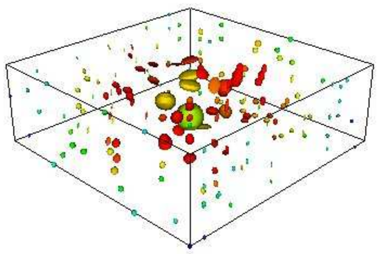

MapOnScalarClipWithRotation

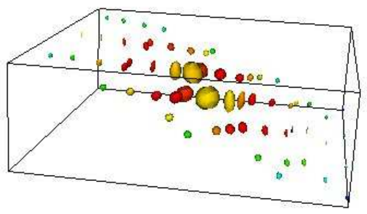

Streamline

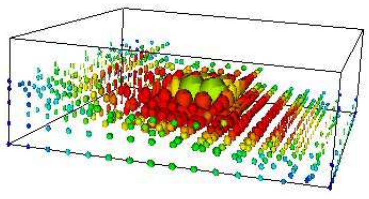

Velocity

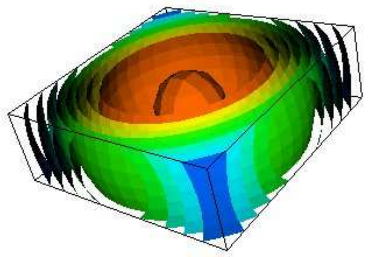

VelocityOnPlaneCut

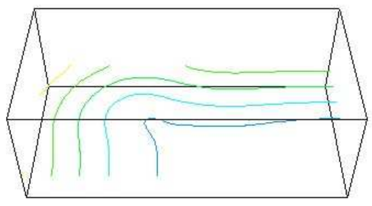

VelocityOnPlaneClip

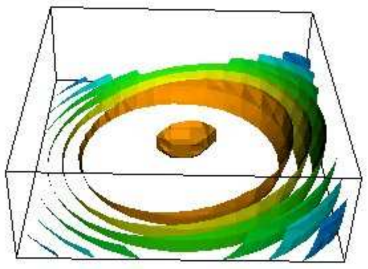

Ellipsoid

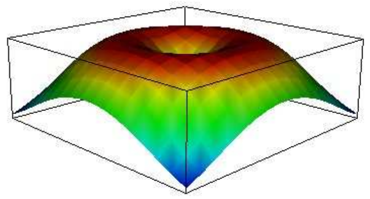

EllipsoidOnPlaneCut

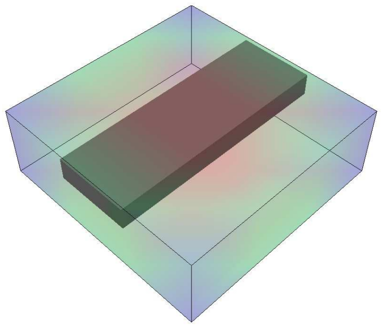

EllipsoidOnPlaneClip

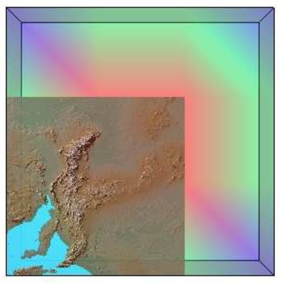

Contour


ContourOnPlaneCut

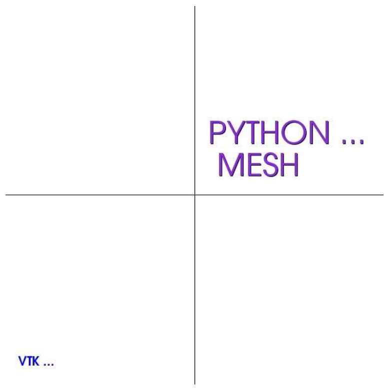

ContourOnPlaneClip


Carpet


Rectangle

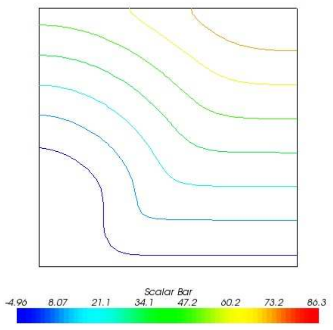


Image



Text

ACCESS
Australian Computational Earth Systems Simulator
MAJOR NATIONAL RESEARCH FACILITY
Logo



Legend

CHAPTER

SEVEN

Models

The following sections give a breif overview of the model classes and their corresponding methods.

7.1 Stokes Problem

The velocity field v and pressure p of an incompressible fluid is given as the solution of the Stokes problem

$$-\left(\eta(v_{i,j}+v_{i,j})\right)_{,j}+p_{,i}=f_i-\sigma_{ij,j} \tag{7.1}$$

where η is the viscosity, F_i defines an internal force and σ_{ij} is an intial stress . We assume an incompressible media:

$$-v_{i,i}=0 \tag{7.2}$$

Natural boundary conditions are taken in the form

$$\left(\eta(v_{i,j}+v_{i,j})\right)n_j-n_ip=s_i+\sigma_{ij}n_i \tag{7.3}$$

which can be overwritten by constraints of the form

$$v_i(x)=v_i^D(x) \tag{7.4}$$

at some locations x at the boundary of the domain. The index i may depend on the location x on the boundary. v^D is a given function on the domain.

7.1.1 Solution Method

In block form equation equations 7.1 and 7.2 takes the form of a saddle point problem

$$\left[\begin{array}{cc} A & B^* \\ B & 0 \end{array}\right]\left[\begin{array}{c} v \\ p \end{array}\right]=\left[\begin{array}{c} G \\ 0 \end{array}\right] \tag{7.5}$$

where A is coercive, self-adjoint linear operator in a suitable Hilbert space, B is the $(-1)\cdot$ divergence operator and B^* is it adjoint operator (=gradient operator). For more details on the mathematics see references [5, 6]. We use iterative techniques to solve this problem. To make sure that the incomressibilty condition holds with sufficient accuracy we check for

$$\|v_{k,k}\|_{\le}\epsilon\|\sqrt{v_{j,k}v_{j,k}}\| \tag{7.6}$$

where ϵ is the desired relative accuracy and

$$\|p\|^2=\int_\Omega p^2\;dx \tag{7.7}$$

defines the L^2-norm. There are two approaches to solve this problem. The first approach, called the Uzawa scheme eliminates the velocity v from the problem. The second approach solves the equation in coupled form after the application of a preconditioner.

Uzawa scheme

The first eqution in 7.5 gives $v = A^{-1}(G - B^*p)$ assuming p is known. This is inserted into the second eqution which leads to

$$Sp = BA^{-1}G \tag{7.8}$$

with the Schur complement $S = BA^{-1}B^*$. This problem can be solved iteratively using the reconditioned Conjugate Gradient Method (PCG) with the preconditioner $\hat{S}$ defined as $q = \hat{S}^{-1}p$ by solving

$$\frac{1}{\eta}q = p \tag{7.9}$$

see [**?**] for more details. The evaluation of $w = Sp$ is done in the form

$$\begin{array}{rcl} Av & = & B^*p \\ w & = & Bv \end{array} \tag{7.10}$$

The residual $r = BA^{-1}G - Sp$ is given as

$$r = BA^{-1}(G - B^*p) = Bv \text{ with } v = A^{-1}(G - B^*p) \tag{7.11}$$

Therefore one uses the tuple (v, Bv) to represent the residual of the current pressure p. Notice that before the iteration is started the right hand side $BA^{-1}G$ needs to be calculated. The bilinear form $(.,.)$ used is defined as

$$(p, (v, Bv)) = \int_\Omega p \cdot Bv \; dx \tag{7.12}$$

where p is the pressure increment and (v, Bv) represents an increment in the residual.

Coupled Solver

An alternative approach to solve the saddle point problem 7.5 directly using an iterative such as the generalized minimal residual method (GMRES) with a suitable preconditioner. Here we use the operator

$$\begin{bmatrix} A^{-1} & 0 \\ S^{-1}BA^{-1} & -S^{-1} \end{bmatrix} \tag{7.13}$$

where again S is the Schur complement [**?**]. In partice we will use an approximation $\hat{S}$ for S. The evaluation (w, q) of the iteration operator for a given (v, p) is done as

$$\begin{array}{rcl} Aw & = & Av + B^*p \\ \hat{S}q & = & B(w - v) \end{array} \tag{7.14}$$

We use the inner product induced by the norm

$$\|(v,p)\|^2 = \int_\Omega v_{i,j}v_{i,j} + \left(\frac{p}{\eta}\right)^2 \; dx \tag{7.15}$$

In PDE form 7.14 takes the form

$$\begin{array}{rcl} -\left(\eta(w_{i,j} + w_{i,j})\right)_{,j} & = & -\left(\eta(v_{i,j} + v_{i,j})\right)_{,j} + p_{,i} \\ \frac{1}{\eta}q & = & -(w - v)_{i,i} \end{array} \tag{7.16}$$

7.1.2 Functions

class `StokesProblemCartesian`(*domain*)

opens the Stokes problem on the `Domain` domain. The approximation order needs to be two.

`initialize`([*f=Data()*, [*fixed_u_mask=Data()*, [*eta=1*, [*surface_stress=Data()*, [*stress=Data()*]]]]])

assigns values to the model parameters. In any call all values must be set. f defines the external force f, *eta* the viscosity η, *surface_stress* the surface stress s and *stress* the initial stress σ. The locations and compontents where the velocity is fixed are set by the values of *fixed_u_mask*. The method will try to cast the given values to appropriate `Data` class objects.

solve(*v,p,* [*max_iter=20,* [*verbose=False,* [*useUzawa=True*]]])
: solves the problem and return approximations for velocity and pressure. The arguments *v* and *p* define initial guess. The values of *v* marked by *fixed_u_mask* remain unchanged. If *useUzawa* is set to `True` the Uzawa scheme is used. Otherwise the problem is solved in coupled form. In most cases the Uzawa scheme is more efficient. *max_iter* defines the maximum number of iteration steps. If *verbose* is set to `True` informations on the progress of of the solver are printed.

setTolerance([*tolerance=1.e-8*])
: sets the tolerance in an appropriate norm relative to the right hand side. The tolerance must be non-negative and less than 1.

getTolerance()
: returns the current relative tolerance.

setAbsoluteTolerance([*tolerance=0.*])
: sets the absolute tolerance for the error in the relevant norm. The tolerance must be non-negative. Typically the absolute talerance is set to 0.

getAbsoluteTolerance()
: sreturns the current absolute tolerance.

setSubToleranceReductionFactor([*reduction=None*])
: sets the reduction factor for the tolerance used to solve the PDEs. A reduction factor in the order of one will minimize compute time per iteration step but my slow down convergence or even lead to divergency. On the other hand a very small value for the PDE tolerance could result in a wast of compute time. If *reduction* is set to *None* the sub-tolerance is solved adaptively but in cases a very small tolerance is set ($< 10^{-6}$) it is recommended to set the reduction factor by hand. This may require some experiments.

getSubToleranceReductionFactor()
: return the current reduction factor for the sub-problem tolerance.

7.1.3 Example: Lit Driven Cavity

The following script ‘lit_driven_cavity.py’ which is available in the example directory illustrates the usage of the `StokesProblemCartesian` class to solve the lit driven cavity problem [**?**]:

```
from esys.escript import *
from esys.finley import Rectangle
from esys.escript.models import StokesProblemCartesian
NE=25
dom = Rectangle(NE,NE,order=2)
x = dom.getX()
sc=StokesProblemCartesian(dom)
mask= (whereZero(x[0])*[1.,0]+whereZero(x[0]-1))*[1.,0] + \
      (whereZero(x[1])*[0.,1.]+whereZero(x[1]-1))*[1.,1]
sc.initialize(eta=.1, fixed_u_mask= mask)
v=Vector(0.,Solution(dom))
v[0]+=whereZero(x[1]-1.)
p=Scalar(0.,ReducedSolution(dom))
v,p=sc.solve(v,p, verbose=True)
saveVTK("u.xml",velocity=v,pressure=p)
```

7.2 Darcy Flux

We want to calculate the velocity u and pressure p on a domain Ω solving the Darcy flux problem

$$\begin{aligned} u_i + \kappa_{ij} p_{,j} &= g_i \\ u_{k,k} &= f \end{aligned} \tag{7.17}$$

with the boundary conditions

$$\begin{aligned} u_i \, n_i = u_i^N \, n_i \quad &\text{on} \quad \Gamma_N \\ p = p^D \quad &\text{on} \quad \Gamma_D \end{aligned} \tag{7.18}$$

where Γ_N and Γ_D are a partition of the boundary of Ω with Γ_D non empty, n_i is the outer normal field of the boundary of Ω, u_i^N and p^D are given functions on Ω, g_i and f are given source terms and κ_{ij} is the given permability. We assume that κ_{ij} is symmetric (which is not really required) and positive definite, i.e there are positive constants α_0 and α_1 wich are independent from the location in Ω such that

$$\alpha_0 \; x_i x_i \leq \kappa_{ij} x_i x_j \leq \alpha_1 \; x_i x_i \tag{7.19}$$

for all x_i.

7.2.1 Solution Method

Without loss of generality we can assume that $u_i^N \; n_i = 0$ and p^D. Otherewise one solves for $u - u^N$ and $p - p^D$ and sets

$$\begin{array}{rcl} g_i & \leftarrow & g_i - u_i^N - \kappa_{ij} p_{,j}^D \\ f & \leftarrow & f - u_{k,k}^N \end{array} \tag{7.20}$$

We set

$$V = \{q \in H^1(\Omega) : q = 0 \text{ on } \Gamma_D\} \tag{7.21}$$

and

$$W = \{v \in (L^2(\Omega))^d : v_{k,k} \in L^2(\Omega) \text{ and } u_i \; n_i = 0 \text{ on } \Gamma_N\} \tag{7.22}$$

and define the operator $Q : V \to (L^2(\Omega))^d$ defined by

$$(Qp)_i = \kappa_{ij} p_{,j} \tag{7.23}$$

and the operator $D : W \to L^2(\Omega)$ defined by

$$Dv = v_{k,k} \tag{7.24}$$

In operator notation the Darcy problem 7.17 is written in the form

$$\begin{array}{rcl} u + Qp & = & g \\ Du & = & f \end{array} \tag{7.25}$$

We solve this equation by minimising the functional

$$J(u,p) := \|u + Qp - g\|_0^2 + \|Du - f\|_0^2 \tag{7.26}$$

over $W \times V$ where $\|.\|_0$ denotes the norm in $L^2(\Omega)$. A simple calculation shows that one has to solve

$$(v + Qq, u + Qp - g) + (Dv, Du - f) = 0 \tag{7.27}$$

for all $v \in W$ and $q \in V$.which translates back into operator notation

$$\begin{array}{rcl} (I + D^*D)u + Qp & = & D^*f + g \\ Q^*u + Q^*Qp & = & Q^*g \end{array} \tag{7.28}$$

where D^* and Q^* denote the adjoint operators. In [**?**] it has been shown that this problem is continuous and coercive in $W \times V$ and therefore has a unique solution. Also standart FEM methods can be used for discretization. It is also possible to solve the problem is coupled form, however this approach leads in some cases to a very ill-conditioned stiffness matrix in particular in the case of a very small or large permability ($\alpha_1 \ll 1$ or $\alpha_0 \gg 1$)

The approach we are taking is to eliminate the velocity u from the problem. Assuming that p is known we have

$$v = (I + D^*D)^{-1}(D^*f + g - Qp) \tag{7.29}$$

(notice that $(I + D^*D)$ is coercive in W) which is inserted into the second equation

$$Q^*(I + D^*D)^{-1}(D^*f + g - Qp) + Q^*Qp = Q^*g \tag{7.30}$$

which is

$$Q^*(I - (I + D^*D)^{-1})Qp = Q^*(g - (I + D^*D)^{-1}(D^*f + g)) \tag{7.31}$$

We use the PCG method to solve this. The residual r ($\in V^*$) is given as

$$\begin{aligned} r &= Q^*(g-(I+D^*D)^{-1}(D^*f+g)-Qp+(I+D^*D)^{-1}Qp \\ &= Q^*\left((g-Qp)-(I+D^*D)^{-1}(D^*f+g-Qp)\right) \\ &= Q^*\left((g-Qp)-v\right) \end{aligned} \tag{7.32}$$

So in a partical implementation we use the pair $(g-Qp,v)$ to represent the residual. This will save the reconstruction of the velocity v. In this notation the right hand side is given as $(g,(I+D^*D)^{-1}(D^*f+g))$. The evaluation of the iteration operator for a given p is then returning (Qp,w) where w is the solution of

$$(I+D^*D)w = Qp \tag{7.33}$$

We use Q^*Q as a a preconditioner for the iteration operator $Q^*(I-(I+D^*D)^{-1})Q$.

7.2.2 Functions

class **`DarcyFlow`**`(`*domain*`)`

opens the Darcy flux problem on the `Domain` domain.

`initialize``(`[*f=Data(),* [*fixed_u_mask=Data(),* [*eta=1,* [*surface_stress=Data(),* [*stress=Data()*]]]]]`)`

assigns values to the model parameters. In any call all values must be set. *f* defines the external force f, *eta* the viscosity η, *surface_stress* the surface stress s and *stress* the initial stress σ. The locations and compontents where the velocity is fixed are set by the values of *fixed_u_mask*. The method will try to cast the given values to appropriate `Data` class objects.

7.2.3 Example: Gravity Flow

7.3 Temperature Advection Diffusion

$$\rho c_p \left(\frac{\partial T}{\partial t} + \vec{v}\cdot\nabla T\right) = k\nabla^2 T \tag{7.34}$$

where $\vec{v}$ is the velocity vector, T is the temperature, ρ is the density, η is the viscosity, c_p is the specific heat at constant pressure and k is the thermal conductivity.

7.3.1 Description

7.3.2 Method

class **`TemperatureCartesian`**`(`*dom,theta=THETA,useSUPG=SUPG*`)`

7.3.3 Benchmark Problem

7.4 Isotropic Kelvin Material

As proposed by Kelvin **??** material strain $D_{ij}=v_{i,j}+v_{j,i}$ can be decomposed into an elastic part D_{ij}^{el} and visco-plastic part D_{ij}^{vp}:

$$D_{ij} = D_{ij}^{el} + D_{ij}^{vp} \tag{7.35}$$

with the elastic strain given as

$$D_{ij}'^{el} = \frac{1}{2\mu}\dot{\sigma}_{ij}' \tag{7.36}$$

where σ_{ij}' is the deviatoric stress (Notice that $\sigma_{ii}'=0$). If the material is composed by materials q the visco-plastic strain can be decomposed as

$$D_{ij}'^{vp} = \sum_q D_{ij}'^{q} \tag{7.37}$$

where D^q_{ij} is the strain in material q given as

$$D'^q_{ij} = \frac{1}{2\eta^q}\sigma'_{ij} \tag{7.38}$$

where η^q is the viscosity of material q. We assume the following betwee the the strain in material q

$$\eta^q = \eta^q_N \left(\frac{\tau}{\tau^q_t}\right)^{\frac{1}{n^q}-1} \text{ with } \tau = \sqrt{\frac{1}{2}\sigma'_{ij}\sigma'_{ij}} \tag{7.39}$$

for a given power law coefficients n^q and transition stresses τ^q_t, see **??**. Notice that $n^q = 1$ gives a constant viscosity. After inserting equation 7.38 into equation 7.37 one gets:

$$D'^{vp}_{ij} = \frac{1}{2\eta^{vp}}\sigma'_{ij} \text{ with } \frac{1}{\eta^{vp}} = \sum_q \frac{1}{\eta^q} \ . \tag{7.40}$$

With

$$\dot{\gamma} = \sqrt{2D_{ij}D_{ij}} \tag{7.41}$$

one gets

$$\tau = \eta^{vp}\dot{\gamma}^{vp} \ . \tag{7.42}$$

With the Drucker-Prager cohesion factor τ_Y, Drucker-Prager friction β and total pressure p we want to achieve

$$\tau \le \tau_Y + \beta\ p \tag{7.43}$$

which leads to the condition

$$\eta^{vp} \le \frac{\tau_Y + \beta\ p}{\dot{\gamma}^{vp}} \ . \tag{7.44}$$

Therefore we modify the definition of η^{vp} to the form

$$\frac{1}{\eta^{vp}} = \max(\sum_q \frac{1}{\eta^q}, \frac{\dot{\gamma}^{vp}}{\tau_Y + \beta\ p}) \tag{7.45}$$

The deviatoric stress needs to fullfill the equilibrion equation

$$-\sigma'_{ij,j} + p_{,i} = F_i \tag{7.46}$$

where F_j is a given external fource. We assume an incompressible media:

$$-v_{i,i} = 0 \tag{7.47}$$

Natural boundary conditions are taken in the form

$$\sigma'_{ij}n_j - n_i p = f \tag{7.48}$$

which can be overwritten by a constraint

$$v_i(x) = 0 \tag{7.49}$$

where the index i may depend on the location x on the bondary.

7.4.1 Solution Method

By using a first order finite difference approximation wit step size $dt > 0$ 7.36 get the form

$$D'^{el}_{ij} = \frac{1}{2\mu dt}\left(\sigma'_{ij} - \sigma'^{-}_{ij}\right) \tag{7.50}$$

where σ'^{-}_{ij} is the deviatoric stress at the precious time step. Now we can combine equations 7.47, 7.50 and 7.45 to get

$$\sigma'_{ij} = 2\eta_{eff}\left(D'_{ij} + \frac{1}{2\mu\ dt}\sigma'^{-}_{ij}\right) \text{ with } \frac{1}{\eta_{eff}} = \frac{1}{\mu\ dt} + \frac{1}{\eta^{vp}} \tag{7.51}$$

Notice that η_{eff} is a function of diatoric stress σ'_{ij}. After inserting 7.51 into 7.46 we get

$$-\left(\eta_{eff}(v_{i,j}+v_{i,j})\right)_{,j} + p_{,i} = F_i + \frac{\eta_{eff}}{\mu dt}\sigma'^{-}_{ij,j} \tag{7.52}$$

Together with the incomressibilty condition 7.47 we need to solve a problem with a form almost identical to the Stokes problem discussed in section 7.1.1 but with the difference that η_{eff} is depending on the solution. Analog to the iteration scheme 7.16 we can run

$$\begin{array}{rcl} -\left(\eta_{eff}(dv_{i,j}+dv_{i,j})\right)_{,j} & = & F_i + \sigma'_{ij,j} - p_{,i} \\ \frac{1}{\eta_{eff}}dp & = & -v^{+}_{i,i} \end{array} \tag{7.53}$$

where $v^{+} = v + dv$. As this problem is non-linear the Jacobi-free Newton-GMRES method is used with the norm

$$\|(v,p)\|^2 = \int_\Omega v_{i,j}^2 + \frac{1}{\bar{\eta}_{eff}^2}p^2 \; dx \tag{7.54}$$

where $\bar{\eta}_{eff}$ is the caracteristic viscosity, for instance:

$$\frac{1}{\bar{\eta}_{eff}} = \frac{1}{\tau^{-}} + \sum_q \frac{1}{\eta_N^q} \tag{7.55}$$

In oder to perform step 7.53 we need to calculate the η_{eff} as well as σ'_{ij} while via τ the first is a function of the latter. The priority is the calculation of η_{eff} with the Newton-Raphson scheme. This value can then be used to calculate σ'_{ij} via 7.51. We need to solve

$$\tau = \eta_{eff}\cdot\epsilon \text{ with } \epsilon = \sqrt{2\left(D'_{ij} + \frac{1}{2\mu\; dt}\sigma'^{-}_{ij}\right)^2} \tag{7.56}$$

The Newton scheme takes the form

$$\tau_{n+1} = \min(\tau_n - \frac{\tau_n - \eta_{eff}\cdot\epsilon}{1-\eta'_{eff}\cdot\epsilon}, \tau_Y + \beta\; p) = \min(\frac{\eta_{eff} - \tau_n\eta'_{eff}}{1-\eta'_{eff}\cdot\epsilon}, \frac{\tau_Y+\beta\; p}{\epsilon})\epsilon \tag{7.57}$$

where η'_{eff} denotes the derivative of η_{eff} with respect of τ. The second term in $\min$ is droped of $\tau_Y + \beta\; p < 0$ or $\epsilon = 0$. In fact we have

$$\eta'_{eff} = -\eta_{eff}^2\left(\frac{1}{\eta_{eff}}\right)' \text{ with } \left(\frac{1}{\eta_{eff}}\right)' = \sum_q\left(\frac{1}{\eta^q}\right)' \tag{7.58}$$

$$\left(\frac{1}{\eta^q}\right)' = \frac{1-\frac{1}{n^q}}{\eta_N^q}\frac{\tau^{-\frac{1}{n^q}}}{(\tau_t^q)^{1-\frac{1}{n^q}}} = \frac{1-\frac{1}{n^q}}{\tau\eta^q} \tag{7.59}$$

Notice that allways $\eta'_{eff} \leq 0$ which makes the denomionator in 7.57 positive.

CHAPTER

EIGHT

The Module `esys.finley`

finley is a library of C functions solving linear, steady partial differential equations (PDEs) or systems of PDEs using isoparametrical finite elements . It supports unstructured, 1D, 2D and 3D meshes. The module `esys.finley` provides an access to the library through the `LinearPDE` class of `esys.escript` supporting its full functionality. *finley* is parallelized using the OpenMP paradigm.

8.1 Formulation

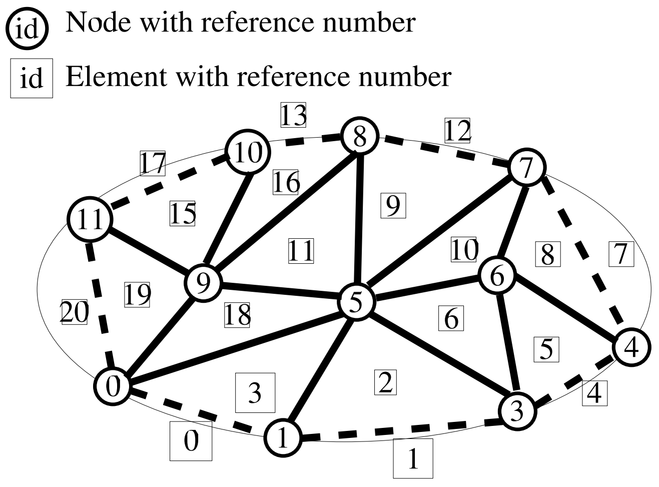
For a single PDE with a solution with a single component the linear PDE is defined in the following form:

$$\begin{array}{rl} & \int_{\Omega} A_{jl} \cdot v_{,j} u_{,l} + B_{j} \cdot v_{,j} u + C_{l} \cdot v u_{,l} + D \cdot v u \; d\Omega \\ + & \int_{\Gamma} d \cdot v u \; d\Gamma + \int_{\Gamma^{contact}} d^{contact} \cdot [v][u] \; d\Gamma \\ = & \int_{\Omega} X_{j} \cdot v_{,j} + Y \cdot v \; d\Omega \\ + & \int_{\Gamma} y \cdot v \; d\Gamma + \int_{\Gamma^{contact}} y^{contact} \cdot [v] \; d\Gamma \end{array} \tag{8.1}$$

8.2 Meshes

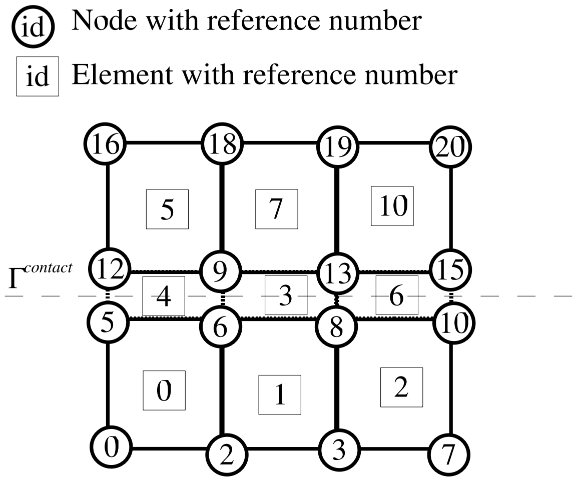
To understand the usage of `esys.finley` one needs to have an understanding of how the finite element meshes are defined. Figure 8.1 shows an example of the subdivision of an ellipse into so called elements . In this case, triangles have been used but other forms of subdivisions can be constructed, e.g. into quadrilaterals or, in the three dimensional case, into tetrahedrons and hexahedrons. The idea of the finite element method is to approximate the solution by a function which is a polynomial of a certain order and is continuous across it boundary to neighbor elements. In the example of Figure 8.1 a linear polynomial is used on each triangle. As one can see, the triangulation is quite a poor approximation of the ellipse. It can be improved by introducing a midpoint on each element edge then positioning those nodes located on an edge expected to describe the boundary, onto the boundary. In this case the triangle gets a curved edge which requires a parametrization of the triangle using a quadratic polynomial. For this case, the solution is also approximated by a piecewise quadratic polynomial (which explains the name isoparametrical elements), see Reference [18, 8] for more details.

The union of all elements defines the domain of the PDE. Each element is defined by the nodes used to describe its shape. In Figure 8.1 the element, which has type *Tri3*, with element reference number 19 is defined by the nodes with reference numbers 9, 11 and 0 . Notice that the order is counterclockwise. The coefficients of the PDE are evaluated at integration nodes with each individual element. For quadrilateral elements a Gauss quadrature scheme is used. In the case of triangular elements a modified form is applied. The boundary of the domain is also subdivided into elements. In Figure 8.1 line elements with two nodes are used. The elements are also defined by their describing nodes, e.g. the face element reference number 20 which has type *Line2* is defined by the nodes with the reference numbers 11 and 0. Again the order is crucial, if moving from the first to second node the domain has to lie on the left hand side (in the case of a two dimension surface element the domain has to lie on the left hand side when moving counterclockwise). If the gradient on the surface of the domain is to be calculated rich face elements face to be used. Rich elements on a face are identical to interior elements but with a modified order



id Node with reference number
id Element with reference number
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

FIGURE 8.1: Subdivision of an Ellipse into triangles order 1 (*Tri3*)



id Node with reference number
id Element with reference number
$\Gamma^{contact}$
16
18
19
20
5
7
10
12
9
13
15
4
3
6
5
6
8
10
0
1
2
0
2
3
7

FIGURE 8.2: Mesh around a contact region (*Rec4*)

of nodes such that the 'first' face of the element aligns with the surface of the domain. In Figure 8.1 elements of the type *Tri3Face* are used. The face element reference number 20 as a rich face element is defined by the nodes with reference numbers 11, 0 and 9. Notice that the face element 20 is identical to the interior element 19 except that, in this case, the order of the node is different to align the first edge of the triangle (which is the edge starting with the first node) with the boundary of the domain.

Be aware that face elements and elements in the interior of the domain must match, i.e. a face element must be the face of an interior element or, in case of a rich face element, it must be identical to an interior element. If no face elements are specified `esys.finley` implicitly assumes homogeneous natural boundary conditions , i.e. d=0 and y=0, on the entire boundary of the domain. For inhomogeneous natural boundary conditions , the boundary must be described by face elements.

If discontinuities of the PDE solution are considered contact elements are introduced to describe the contact region $\Gamma^{contact}$ even if $d^{contact}$ and $y^{contact}$ are zero. Figure 8.2 shows a simple example of a mesh of rectangular elements around a contact region $\Gamma^{contact}$. The contact region is described by the elements 4, 3 and 6. Their element type is *Line2_Contact*. The nodes 9, 12, 6, 5 define contact element 4, where the coordinates of nodes 12 and 5 and nodes 4 and 6 are identical with the idea that nodes 12 and 9 are located above and nodes 5 and 6 below the contact region. Again, the order of the nodes within an element is crucial. There is also the option of

interior	face	rich face	contact	rich contact
Line2	*Point1*	*Line2Face*	*Point1_Contact*	*Line2Face_Contact*
Line3	*Point1*	*Line3Face*	*Point1_Contact*	*Line3Face_Contact*
Tri3	*Line2*	*Tri3Face*	*Line2_Contact*	*Tri3Face_Contact*
Tri6	*Line3*	*Tri6Face*	*Line3_Contact*	*Tri6Face_Contact*
Rec4	*Line2*	*Rec4Face*	*Line2_Contact*	*Rec4Face_Contact*
Rec8	*Line3*	*Rec8Face*	*Line3_Contact*	*Rec8Face_Contact*
Rec9	*Line3*	*Rec9Face*	*Line3_Contact*	*Rec9Face_Contact*
Tet4	*Tri6*	*Tet4Face*	*Tri6_Contact*	*Tet4Face_Contact*
Tet10	*Tri9*	*Tet10Face*	*Tri9_Contact*	*Tet10Face_Contact*
Hex8	*Rec4*	*Hex8Face*	*Rec4_Contact*	*Hex8Face_Contact*
Hex20	*Rec8*	*Hex20Face*	*Rec8_Contact*	*Hex20Face_Contact*

Table 8.1: Finley elements and corresponding elements to be used on domain faces and contacts. The rich types have to be used if the gradient of function is to be calculated on faces and contacts, respectively.

using rich elements if the gradient is to be calculated on the contact region. Similarly to the rich face elements these are constructed from two interior elements by reordering the nodes such that the 'first' face of the element above and the 'first' face of the element below the contact regions line up. The rich version of element 4 is of type *Rec4Face_Contact* and is defined by the nodes 9, 12, 16, 18, 6, 5, 0 and 2.

Table 8.1 shows the interior element types and the corresponding element types to be used on the face and contacts. Figure 8.3, Figure 8.4 and Figure 8.5 show the ordering of the nodes within an element.

The native `esys.finley` file format is defined as follows. Each node *i* has *dim* spatial coordinates *Node[i]*, a reference number *Node_ref[i]*, a degree of freedom *Node_DOF[i]* and tag *Node_tag[i]*. In most cases *Node_DOF[i]=Node_ref[i]* however, for periodic boundary conditions, *Node_DOF[i]* is chosen differently, see example below. The tag can be used to mark nodes sharing the same properties. Element *i* is defined by the *Element_numNodes* nodes *Element_Nodes[i]* which is a list of node reference numbers. The order is crucial. It has a reference number *Element_ref[i]* and a tag *Element_tag[i]*. The tag can be used to mark elements sharing the same properties. For instance elements above a contact region are marked with 2 and elements below a contact region are marked with 1. *Element_Type* and *Element_Num* give the element type and the number of elements in the mesh. Analogue notations are used for face and contact elements. The following Python script prints the mesh definition in the `esys.finley` file format:

```
print "%s\n"%mesh_name
# node coordinates:
print "%dD-nodes %d\n"%(dim,numNodes)
for i in range(numNodes):
   print "%d %d %d"%(Node_ref[i],Node_DOF[i],Node_tag[i])
   for j in range(dim): print " %e"%Node[i][j]
   print "\n"
# interior elements
print "%s %d\n"%(Element_Type,Element_Num)
for i in range(Element_Num):
   print "%d %d"%(Element_ref[i],Element_tag[i])
   for j in range(Element_numNodes): print " %d"%Element_Nodes[i][j]
   print "\n"
# face elements
print "%s %d\n"%(FaceElement_Type,FaceElement_Num)
for i in range(FaceElement_Num):
   print "%d %d"%(FaceElement_ref[i],FaceElement_tag[i])
   for j in range(FaceElement_numNodes): print " %d"%FaceElement_Nodes[i][j]
   print "\n"
# contact elements
print "%s %d\n"%(ContactElement_Type,ContactElement_Num)
for i in range(ContactElement_Num):
   print "%d %d"%(ContactElement_ref[i],ContactElement_tag[i])
   for j in range(ContactElement_numNodes): print " %d"%ContactElement_Nodes[i][j]
   print "\n"
# point sources (not supported yet)
```

```
write("Point1 0",face_element_type,numFaceElements)
```

The following example of a mesh file defines the mesh shown in Figure 8.2:

```
Example 1
2D Nodes 16
0   0 0 0.   0.
2   2 0 0.33 0.
3   3 0 0.66 0.
7   4 0 1.   0.
5   5 0 0.   0.5
6   6 0 0.33 0.5
8   8 0 0.66 0.5
10 10 0 1.0  0.5
12 12 0 0.   0.5
9   9 0 0.33 0.5
13 13 0 0.66 0.5
15 15 0 1.0  0.5
16 16 0 0.   1.0
18 18 0 0.33 1.0
19 19 0 0.66 1.0
20 20 0 1.0  1.0
Rec4 6
 0 1  0  2  6  5
 1 1  2  3  8  6
 2 1  3  7 10  8
 5 2 12  9 18 16
 7 2 13 19 18  9
10 2 20 19 13 15
Line2 0
Line2_Contact 3
 4 0  9 12  6 5
 3 0 13  9  8 6
 6 0 15 13 10 8
Point1 0
```

Notice that the order in which the nodes and elements are given is arbitrary. In the case that rich contact elements are used the contact element section gets the form

```
Rec4Face_Contact 3
 4 0  9 12 16 18  6  5  0  2
 3 0 13  9 18 19  8  6  2  3
 6 0 15 13 19 20 10  8  3  7
```

Periodic boundary condition can be introduced by altering *Node_DOF*. It allows identification of nodes even if they have different physical locations. For instance, to enforce periodic boundary conditions at the face $x0 = 0$ and $x0 = 1$ one identifies the degrees of freedom for nodes 0, 5, 12 and 16 with the degrees of freedom for 7, 10, 15 and 20, respectively. The node section of the `esys.finley` mesh gets now the form:

```
2D Nodes 16
0   0 0 0.   0.
2   2 0 0.33 0.
3   3 0 0.66 0.
7   0 0 1.   0.
5   5 0 0.   0.5
6   6 0 0.33 0.5
8   8 0 0.66 0.5
10  5 0 1.0  0.5
12 12 0 0.   0.5
9   9 0 0.33 0.5
13 13 0 0.66 0.5
15 12 0 1.0  0.5
16 16 0 0.   1.0
18 18 0 0.33 1.0
19 19 0 0.66 1.0
20 16 0 1.0  1.0
```

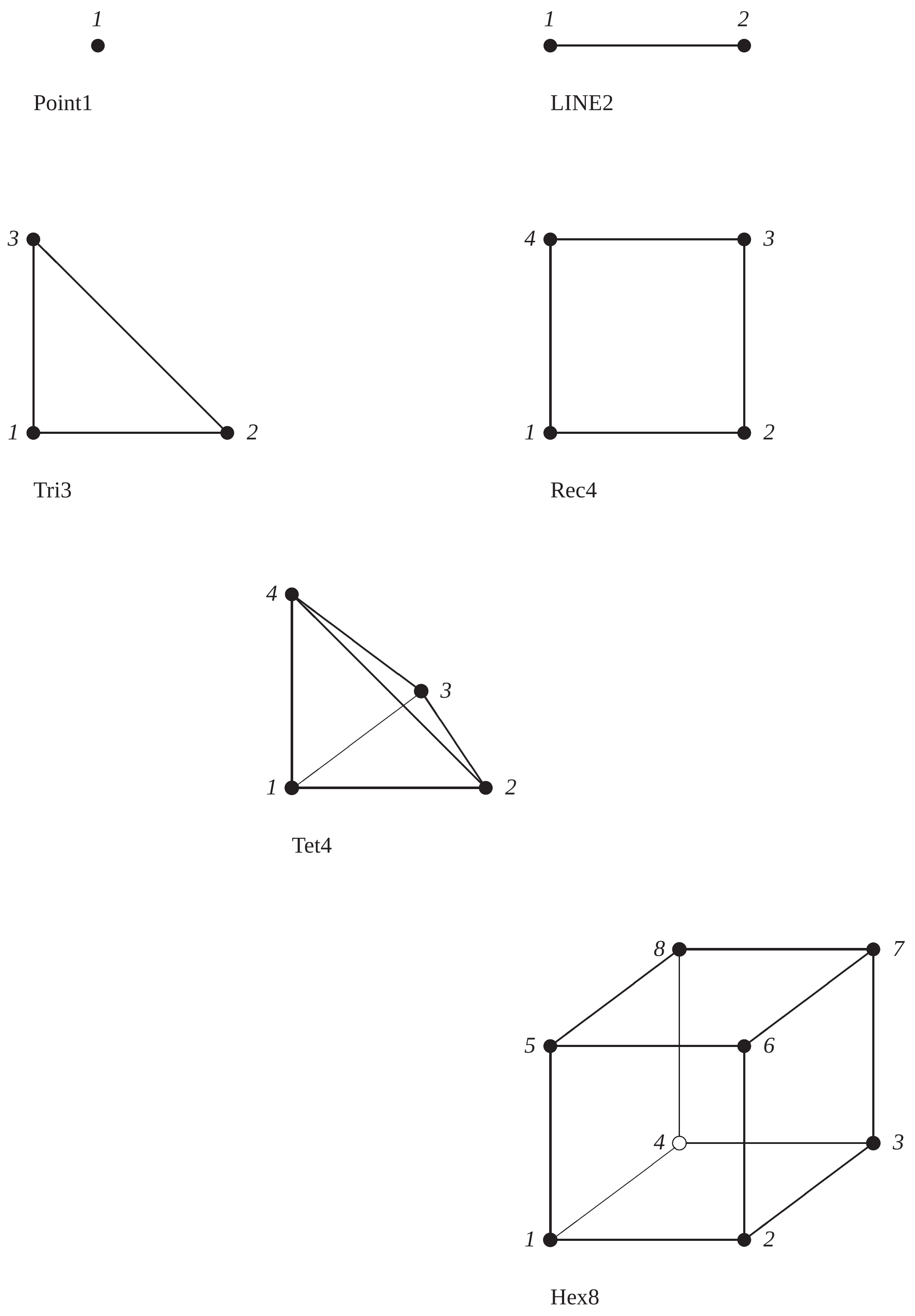


FIGURE 8.3: Elements of order 1

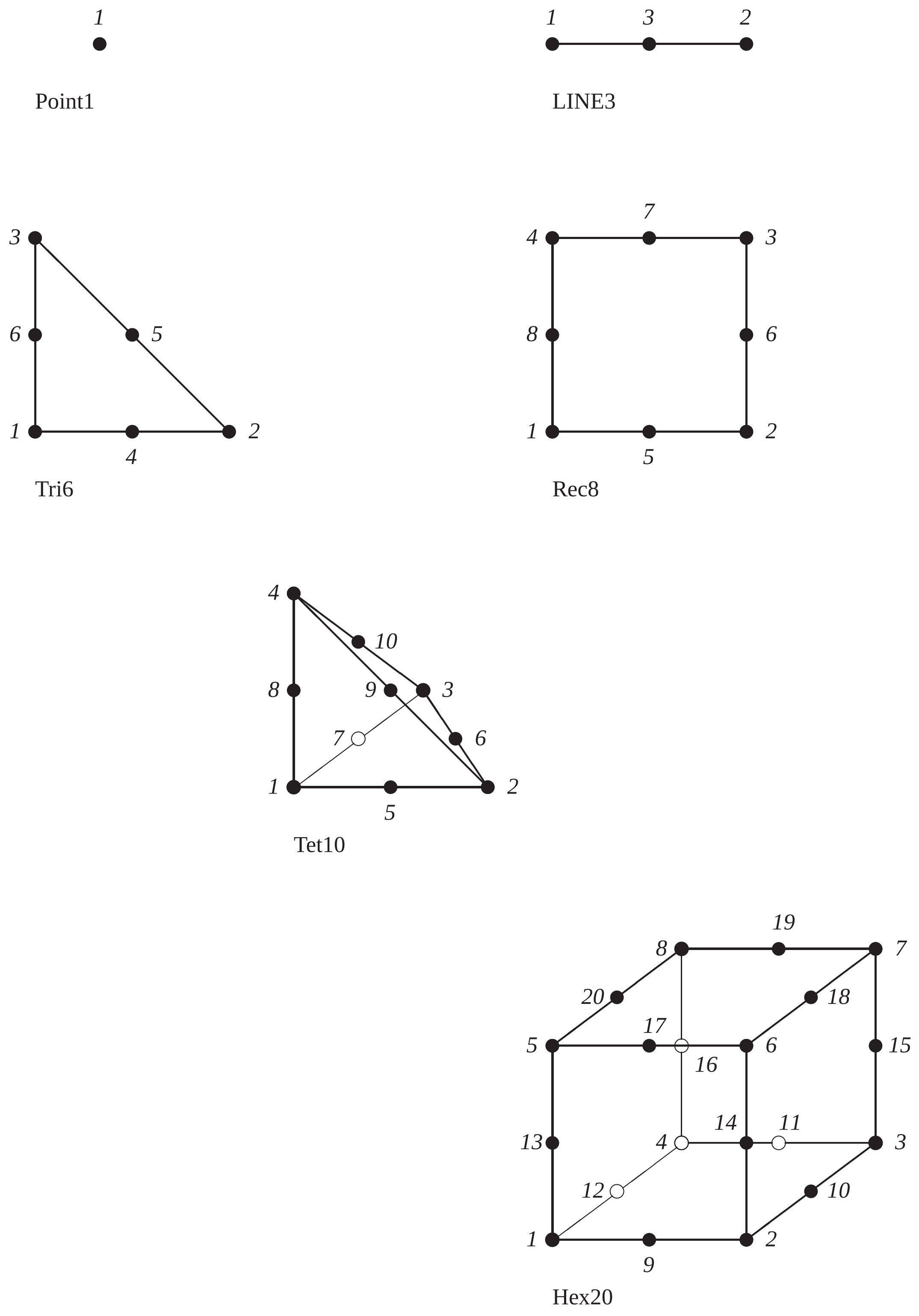


FIGURE 8.4: Elements of order 2

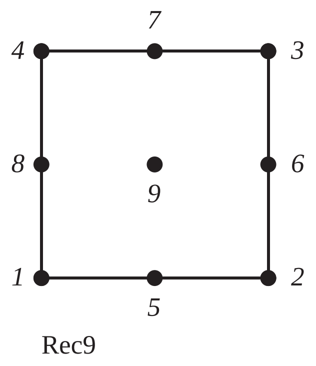


FIGURE 8.5: Additional shape functions

8.2.1 Linear Solvers in `LinearPDE`

Currently `esys.finley` supports the linear solvers `LinearPDE.PCG` , `LinearPDE.GMRES` , `LinearPDE.PRES20` and `LinearPDE.BICGSTAB` . For `LinearPDE.GMRES` the options *truncation* and *restart* of the `getSolution` can be used to control the truncation and restart during iteration. Default values are *truncation*=5 and *restart*=20. The default solver is `LinearPDE.BICGSTAB` but if the symmetry flag is set `LinearPDE.PCG` is the default solver. `esys.finley` supports the solver options *iter_max* which specifies the maximum number of iterations steps, *verbose*=`True` or `False` and *preconditioner*=`JACOBI` or `ILU0`. In some installations `esys.finley` supports the `LinearPDE.DIRECT` solver and the solver options *reordering*=`util.NO_REORDERING`, `util.MINIMUM_FILL_IN` or `util.NESTED_DISSECTION` (default is `util.NO_REORDERING`), *drop_tolerance* specifying the threshold for values to be dropped in the incomplete elimination process (default is 0.01) and *drop_storage* specifying the maximum increase in storage allowed in the incomplete elimination process (default is 1.20).

8.2.2 Functions

`Mesh``(`*fileName,integrationOrder=-1*`)`

creates a `Domain` object form the FEM mesh defined in file *fileName*. The file must be given the `esys.finley` file format. If *integrationOrder* is positive, a numerical integration scheme chosen which is accurate on each element up to a polynomial of degree *integrationOrder* . Otherwise an appropriate integration order is chosen independently.

`Rectangle``(`*n0,n1,order=1,l0=1.,l1=1., integrationOrder=-1, periodic0=*`False`*,periodic1=*`False`*,useElementsOnFace=*`False`*,optimize=*`False``)`

Generates a `Domain` object representing a two dimensional rectangle between $(0,0)$ and $(l0,l1)$ with orthogonal edges. The rectangle is filled with *n0* elements along the $x0$-axis and *n1* elements along the $x1$-axis. For *order*=1 and *order*=2 *Rec4* and *Rec8* are used, respectively. In the case of *useElementsOnFace*=`False`, *Line2* and *Line3* are used to subdivide the edges of the rectangle, respectively. In the case of *useElementsOnFace*=`True` (this option should be used if gradients are calculated on domain faces), *Rec4Face* and *Rec8Face* are used on the edges, respectively. If *integrationOrder* is positive, a numerical integration scheme chosen which is accurate on each element up to a polynomial of degree *integrationOrder* . Otherwise an appropriate integration order is chosen independently. If *periodic0*=`True`, periodic boundary conditions along the $x0$-directions are enforced. That means when for any solution of a PDE solved by `esys.finley` the value on the line $x0 = 0$ will be identical to the values on $x0 =$ *l0*. Correspondingly, *periodic1*=`False` sets periodic boundary conditions in $x1$-direction. If *optimize*=`True` mesh node relabeling will be attempted to reduce the computation and also ParMETIS will be used to improve the mesh partition if running on multiple CPUs with MPI.

`Brick``(`*n0,n1,n2,order=1,l0=1.,l1=1.,l2=1., integrationOrder=-1, periodic0=*`False`*,periodic1=*`False`*,periodic2=*`False`*,useElementsOnFace=*`False`*,optimize=*`False``)`

Generates a `Domain` object representing a three dimensional brick between $(0,0,0)$ and $(l0,l1,l2)$ with orthogonal faces. The brick is filled with *n0* elements along the $x0$-axis, *n1* elements along the $x1$-axis and *n2* elements along the $x2$-axis. For *order*=1 and *order*=2 *Hex8* and *Hex20* are used, respectively. In the case of *useElementsOnFace*=`False`, *Rec4* and *Rec8* are used to subdivide the faces of the brick, respectively. In the case of *useElementsOnFace*=`True` (this option should be used if gradients are calculated on domain faces), *Hex8Face* and *Hex20Face* are used on the brick faces, respectively. If *integrationOrder* is positive, a numerical integration scheme chosen which is accurate on each element up to a polynomial of degree *integrationOrder* . Otherwise an appropriate integration order is chosen independently. If *periodic0*=`True`, periodic boundary conditions along the $x0$-directions are enforced. That means when for any solution of a PDE solved by `esys.finley` the value on the plane $x0 = 0$ will be identical to the values on $x0 =$ *l0*. Correspondingly, *periodic1*=`False` and *periodic2*=`False` sets periodic boundary conditions in $x1$-direction and $x2$-direction, respectively. If *optimize*=`True` mesh node relabeling will be attempted to reduce the computation and also ParMETIS will be used to improve the mesh partition if running on multiple CPUs with MPI.

`GlueFaces``(`*meshList,safetyFactor=0.2,tolerance=1.e-13*`)`

Generates a new `Domain` object from the list *meshList* of `esys.finley` meshes. Nodes in face elements whose difference of coordinates is less then *tolerance* times the diameter of the domain are merged. The corresponding face elements are removed from the mesh.

TODO: explain *safetyFactor* and show an example.

`JoinFaces``(`*meshList,safetyFactor=0.2,tolerance=1.e-13*`)`
Generates a new `Domain` object from the list *meshList* of `esys.finley` meshes. Face elements whose nodes coordinates have difference is less then *tolerance* times the diameter of the domain are combined to form a contact element The corresponding face elements are removed from the mesh.

TODO: explain *safetyFactor* and show an example.

CHAPTER

NINE

Appendix

9.1 Einstein Notation

Compact notation is used in equations such continuum mechanics and linear algebra; it is known as Einstein notation or the Einstein summation convention. It makes the conventional notation of equations involing tensors more compact, by shortening and simplifying them.

There are two rules which make up the convention:

firstly, the rank of the tensor is represented by an index. For example, a is a scalar; b_i represents a vector; and c_{ij} represents a matrix.

Secondly, if an expression contains subscripted variables, they are assumed to be summed over all possible values, from 0 to n. For example, for the following expression:

$$y = a_0 b_0 + a_1 b_1 + \ldots + a_n b_n \tag{9.1}$$

can be represented as:

$$y = \sum_{i=0}^{n} a_i b_i \tag{9.2}$$

then in Einstein notion:

$$y = a_i b_i \tag{9.3}$$

Another example:

$$\nabla p = \frac{\partial p}{\partial x_0}\mathbf{i} + \frac{\partial p}{\partial x_1}\mathbf{j} + \frac{\partial p}{\partial x_2}\mathbf{k} \tag{9.4}$$

can be expressed in Einstein notation as:

$$\nabla p = p_{,i} \tag{9.5}$$

where the comma ',' indicates the partial derivative.

For a tensor:

$$\sigma_{ij} = \begin{bmatrix} \sigma_{00} & \sigma_{01} & \sigma_{02} \\ \sigma_{10} & \sigma_{11} & \sigma_{12} \\ \sigma_{20} & \sigma_{21} & \sigma_{22} \end{bmatrix} \tag{9.6}$$

The δ_{ij} is the Kronecker δ-symbol, which is a matrix with ones for its diagonal entries ($i = j$) and zeros for the remaining entries ($i \neq j$).

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases} \tag{9.7}$$

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