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

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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`
- a model library.

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

Please see Chapter 2 for changes to the way to launch `esys.escript` scripts. For more info on this and other changes from previous releases see Appendix B.

If you use this software in your research, then we would appreciate (but do not require) a citation. Some relevant references can be found in Appendix D.

Researchers and Developers

Escript is the product of years of work by many people. The active researchers for the current release series (3.X) are listed here in alphabetical order. While development is collaborative, each person is listed with some of their major contributions — this list is not exhaustive. Personel for previous release series are listed in an appendix of the user guide.

Cihan Altinay `esys.weipa` visualisation package, SCons build system rework.

Artak Amirbekyan Solvers, OSX work [prior to 3.2.1].

Joel Fenwick Lazy evaluation, maintenance of escript module, release wrangler.

Lin Gao Performance analysis.

Lutz Gross Patriarch, technical lead, solvers, large chunks of the original code.

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ONE

Tutorial: Solving PDEs

1.1 Installation

To download *escript* and friends, please visit `https://launchpad.net/escript-finley`. The web site offers binary distributions for some platforms and provides information about the installation process.

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

1.2 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 in 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

$$-\Delta u = f \tag{1.1}$$

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

$$\Omega = [0,1]^2 = \{(x_0; x_1) | 0 \leq x_0 \leq 1 \text{ and } 0 \leq x_1 \leq 1\} \tag{1.2}$$

The domain is shown in Figure 1.1.

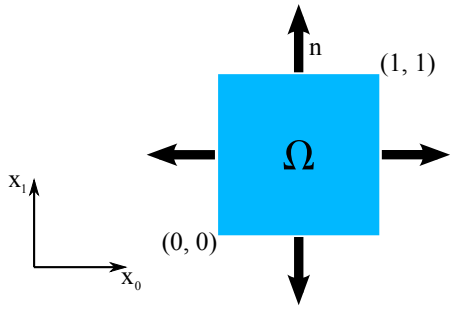


FIGURE 1.1: Domain $\Omega = [0,1]^2$ with outer normal field n.

Δ denotes the Laplace operator, which is defined by

$$\Delta u = (u_{,0})_{,0} + (u_{,1})_{,1} \tag{1.3}$$

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

$$\Delta u = u_{,00} + u_{,11} = \sum_{i=0}^{2} u_{,ii} \tag{1.4}$$

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

$$x_i y_i = \sum_{i=0}^{2} x_i y_i \tag{1.5}$$

$$x_i u_{,i} = \sum_{i=0}^{2} x_i u_{,i} \tag{1.6}$$

$$u_{,ii} = \sum_{i=0}^{2} u_{,ii} \tag{1.7}$$

$$x_{ij} u_{i,j} = \sum_{j=0}^{2} \sum_{i=0}^{2} x_{ij} u_{i,j} \tag{1.8}$$

$$\tag{1.9}$$

With the summation convention we can write the Poisson equation as

$$-u_{,ii} = 1 \tag{1.10}$$

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, i.e. u shall fulfill the homogeneous Neumann boundary condition

$$n_i u_{,i} = 0 \; . \tag{1.11}$$

$n = (n_i)$ denotes the outer normal field of the domain, see Figure 1.1. 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 (1.11) should be fulfilled on the set Γ^N which is the top and right edge of the domain:

$$\Gamma^N = \{(x_0; x_1) \in \Omega | x_0 = 1 \text{ or } x_1 = 1\} \tag{1.12}$$

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

$$\Gamma^D = \{(x_0; x_1) \in \Omega | x_0 = 0 \text{ or } x_1 = 0\} \tag{1.13}$$

the solution shall be identical to zero:

$$u = 0 \; . \tag{1.14}$$

This kind of boundary condition is called a homogeneous Dirichlet boundary condition. The partial differential equation in Equation (1.10) together with the Neumann boundary condition Equation (1.11) and Dirichlet boundary condition in Equation (1.14) form a so-called boundary value problem (BVP) for the unknown function u.

[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 (1.1) as

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

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

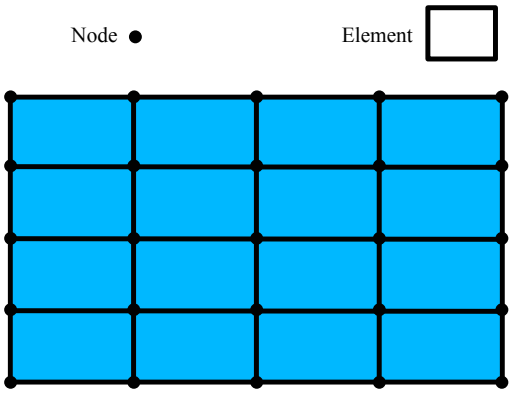


FIGURE 1.2: Mesh of 4×4 elements on a rectangular domain. Here each element is a quadrilateral and described by four nodes, namely the corner points. The solution is interpolated by a bi-linear polynomial.

In general the BVP cannot be solved analytically and numerical methods have to be used to 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 their connection through elements is called a mesh. Figure 1.2 shows an example of a FEM mesh with four elements in the x_0 and four elements in the x_1 direction over the unit square. For more details we refer the reader to the literature, for instance Reference [38, 4].

The `esys.escript` solver we want to use to solve this problem is embedded into the python interpreter language. So you can solve the problem interactively but you will learn quickly that it is more efficient to use scripts which you can edit with your favorite editor. To enter the escript environment, use the **`run-escript`** command[3]:

```
run-escript
```

which will pass you on to the python prompt

```
Python 2.5.2 (r252:60911, Oct  5 2008, 19:29:17)
[GCC 4.3.2] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Here you can use all available python commands and language features, for instance

```
>>> x=2+3
>>> print "2+3=",x
2+3= 5
```

We refer to the python user's guide if you not familiar with python.

`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`:

```
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 $(\texttt{l0},\texttt{l1}) = (1,1)$. 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 7.

[3] **`run-escript`** is not available under Windows yet. If you run under Windows you can just use the **`python`** command and the **OMP_NUM_THREADS** environment variable to control the number of threads.

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 (1.11). 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 (1.13), 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 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 a function which equals 1 where `x[0]` is (almost) equal to zero and 0 elsewhere. Similarly, `whereZero(x[1])` creates a 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 the homogeneous Dirichlet boundary condition is set. The complete definition of our example is now:

```
from esys.escript.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. To get the solution of the Poisson equation defined by `mypde` we just have to call its `getSolution` method.

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()
```

The question is what we do with the calculated solution `u`. Besides postprocessing, e.g. calculating the gradient or the average value, which will be discussed later, plotting the solution is one of the things you might want to do. `esys.escript` offers two ways to do this, both based on external modules or packages and so data need to converted to hand over the solution. The first option is using the `matplotlib` module which allows plotting 2D results relatively quickly from within the Python script, see [14]. However, there are limitations when using this tool, especially for large problems and when solving 3-dimensional problems. Therefore, `esys.escript` provides functionality to export data as files which can subsequently be read by third-party software packages such as *mayavi* [16] or *VisIt* [34].

1.2.1 Plotting Using `matplotlib`

The `matplotlib` module provides a simple and easy-to-use way to visualize PDE solutions (or other `Data` objects). To hand over data from `esys.escript` to `matplotlib` the values need to mapped onto a rectangular grid[4]. We will make use of the `numpy` module.

First we need to create a rectangular grid which is accomplished by the following statements:

```
import numpy
x_grid = numpy.linspace(0., 1., 50)
y_grid = numpy.linspace(0., 1., 50)
```

`x_grid` is an array defining the x coordinates of the grid while `y_grid` defines the y coordinates of the grid. In this case we use 50 points over the interval $[0, 1]$ in both directions.

Now the values created by `esys.escript` need to be interpolated to this grid. We will use the `matplotlib` `mlab.griddata` function to do this. Spatial coordinates are easily extracted as a `list` by

```
x=mydomain.getX()[0].toListOfTuples()
y=mydomain.getX()[1].toListOfTuples()
```

In principle we can apply the same `toListOfTuples` method to extract the values from the PDE solution `u`. However, we have to make sure that the `Data` object we extract the values from uses the same `FunctionSpace` as we have used when extracting `x` and `y`. We apply the `interpolation` to `u` before extraction to achieve this:

```
z=interpolate(u, mydomain.getX().getFunctionSpace())
```

The values in `z` are the values at the points with the coordinates given by `x` and `y`. These values are interpolated to the grid defined by `x_grid` and `y_grid` by using

[4]Users of Debian 5 (Lenny) please note: this example makes use of the `griddata` method in `matplotlib.mlab`. This method is not part of version 0.98.1 which is available with Lenny. If you wish to use contour plots, you may need to install a later version. Users of Ubuntu 8.10 or later should be fine.

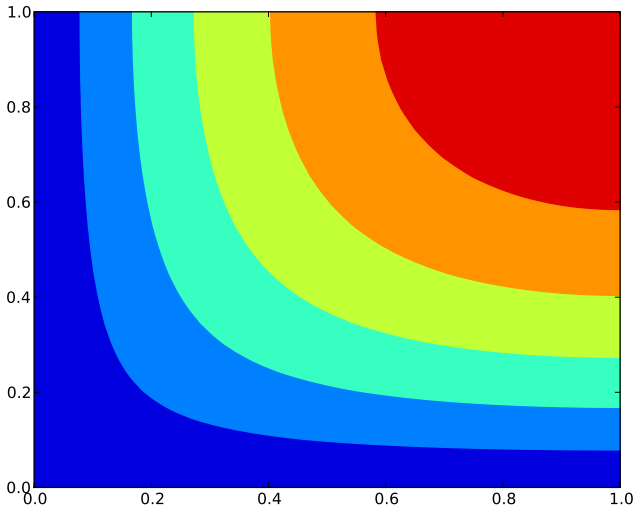


FIGURE 1.3: Visualization of the Poisson Equation Solution for $f = 1$ using `matplotlib`

```
import matplotlib
z_grid = matplotlib.mlab.griddata(x, y, z, xi=x_grid, yi=y_grid)
```

Now `z_grid` gives the values of the PDE solution `u` at the grid which can be plotted using `contourf`:

```
matplotlib.pyplot.contourf(x_grid, y_grid, z_grid, 5)
matplotlib.pyplot.savefig("u.png")
```

Here we use 5 contours. The last statement writes the plot to the file `u.png` in the PNG format. Alternatively, one can use

```
matplotlib.pyplot.contourf(x_grid, y_grid, z_grid, 5)
matplotlib.pyplot.show()
```

which gives an interactive browser window.

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
import numpy
import matplotlib
import pylab
# 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()
# interpolate u to a matplotlib grid:
x_grid = numpy.linspace(0.,1.,50)
y_grid = numpy.linspace(0.,1.,50)
x=mydomain.getX()[0].toListOfTuples()
y=mydomain.getX()[1].toListOfTuples()
z=interpolate(u,mydomain.getX().getFunctionSpace())
z_grid = matplotlib.mlab.griddata(x,y,z,xi=x_grid,yi=y_grid )
```

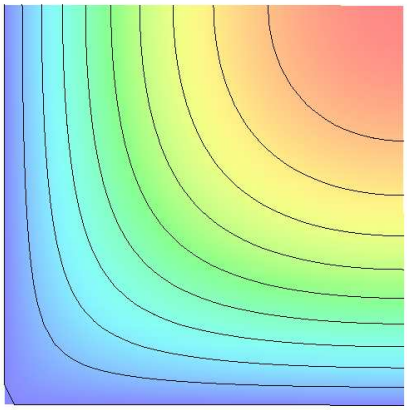


FIGURE 1.4: Visualization of the Poisson Equation Solution for $f = 1$

```
# interpolate u to a rectangular grid:
matplotlib.pyplot.contourf(x_grid, y_grid, z_grid, 5)
matplotlib.pyplot.savefig("u.png")
```

The entire code is available as `poisson_matplotlib.py` in the example directory. You can run the script using the *escript* environment

```
run-escript poisson_matplotlib.py
```

This will create the `u.png`, see Figure 1.3. For details on the usage of the `matplotlib` module we refer to the documentation [14].

As pointed out, `matplotlib` is restricted to the two-dimensional case and should be used for small problems only. It can not be used under *MPI* as the `toListOfTuples` method is not safe under *MPI*[5].

1.2.2 Visualization using export files

As an alternative to `matplotlib`, *escript* supports exporting data to *VTK* and *SILO* files which can be read by visualization tools such as mayavi[16] and *VisIt* [34]. This method is *MPI* safe and works with large 2D and 3D problems.

To write the solution `u` of the Poisson problem in the *VTK* file format to the file `u.vtu` one needs to add:

```
from esys.weipa import saveVTK
saveVTK("u.vtu", sol=u)
```

This file can then be opened in a *VTK* compatible visualization tool where the solution is accessible by the name *sol*. Similarly,

```
from esys.weipa import saveSilo
saveSilo("u.silo", sol=u)
```

will write `u` to a *SILO* file if escript was compiled with *SILO* support.

The Poisson problem script is now

```
from esys.escript import *
from esys.escript.linearPDEs import Poisson
from esys.finley import Rectangle
from esys.weipa import saveVTK
```

[5]The phrase 'safe under *MPI*' means that a program will produce correct results when run on more than one processor under *MPI*.

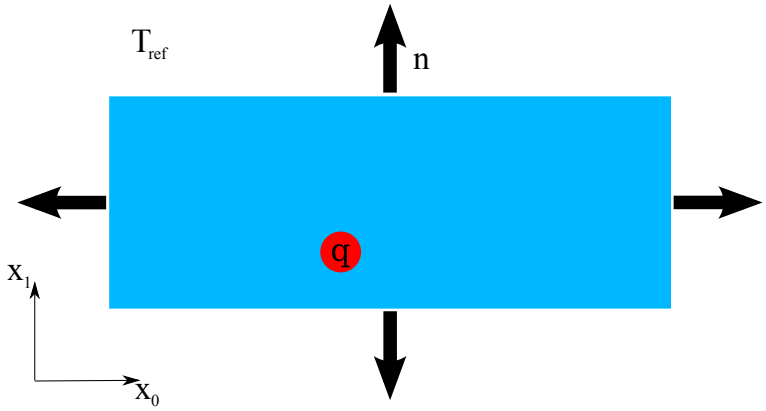


FIGURE 1.5: Temperature Diffusion Problem with Circular Heat Source

```
# 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.vtu",sol=u)
```

The entire code is available as `poisson_vtk.py` in the example directory.

You can run the script using the *escript* environment and visualize the solution using *mayavi*:

```
run-escript poisson_vtk.py
mayavi2 -d u.vtu -m SurfaceMap
```

The result is shown in Figure 1.4.

1.3 The Diffusion Problem

1.3.1 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 1.5 shows the configuration.

In the next Section 1.3.2 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 1.3.3. In Section 1.3.4 this solver is used to build a solver for the temperature diffusion problem.

1.3.2 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

$$\rho c_p T_{,t} - (\kappa T_{,i})_{,i} = q_H \tag{1.15}$$

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 1.2. 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:

$$q_H(x,t) = \begin{cases} q^c & \text{if } \|x - x^c\| \leq r \\ 0 & \text{else} \end{cases} \tag{1.16}$$

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

On the surface of the domain we specify 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}:

$$\kappa T_{,i} n_i = \eta(T_{ref} - T) \tag{1.17}$$

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 (1.15) the initial temperature at time $t = 0$ has to be given. Here we assume that the initial temperature is the surrounding temperature:

$$T(x,0) = T_{ref} \tag{1.18}$$

for all x in the domain. Note that the initial conditions satisfy the boundary condition defined by Equation (1.17).

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 temperature is the backward Euler scheme. The backward Euler scheme is based on the Taylor expansion of T at time $t^{(n)}$:

$$T^{(n)} \approx T^{(n-1)} + T^{(n)}_{,t}(t^{(n)} - t^{(n-1)}) = T^{(n-1)} + h \cdot T^{(n)}_{,t} \tag{1.19}$$

This is inserted into Equation (1.15). By separating the terms at $t^{(n)}$ and $t^{(n-1)}$ one gets for $n = 1, 2, 3 \ldots$

$$\frac{\rho c_p}{h} T^{(n)} - (\kappa T^{(n)}_{,i})_{,i} = q_H + \frac{\rho c_p}{h} T^{(n-1)} \tag{1.20}$$

where $T^{(0)} = T_{ref}$ is taken form the initial condition given by Equation (1.18). Together with the natural boundary condition

$$\kappa T^{(n)}_{,i} n_i = \eta(T_{ref} - T^{(n)}) \tag{1.21}$$

taken from Equation (1.17) 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 implement a solver for the boundary value problem that has to be solved at each time step.

1.3.3 Helmholtz Problem

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

$$\omega T^{(n)} - (\kappa T^{(n)}_{,i})_{,i} = f \tag{1.22}$$

and we set

$$\omega = \frac{\rho c_p}{h} \text{ and } f = q_H + \frac{\rho c_p}{h} T^{(n-1)} \, . \tag{1.23}$$

With $g = \eta T_{ref}$ the radiation condition defined by Equation (1.21) takes the form

$$\kappa T^{(n)}_{,i} n_i = g - \eta T^{(n)} \text{ on } \Gamma \tag{1.24}$$

The partial differential Equation (1.22) together with boundary conditions of Equation (1.24) 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:

$$-(A_{jl} u_{,l})_{,j} + Du = Y \tag{1.25}$$

where we show only the coefficients relevant for the problem discussed here. For the general form of a 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:

$$n_j A_{jl} u_{,l} + du = y \ . \tag{1.26}$$

Notice that the coefficient A is the same like in the PDE Equation (1.25). The coefficients d and y are each a scalar `Data` object in the boundary `FunctionSpace`. Constraints for the solution prescribe the value of the solution at certain locations in the domain. They have the form

$$u = r \text{ where } q > 0 \tag{1.27}$$

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 (1.27) override any other condition set by Equation (1.25) or Equation (1.26). The `Poisson` class of the `esys.escript.linearPDEs` module, which we have already used in Chapter 1.2, 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 (1.22) and boundary condition (1.24), and substituting u for $T^{(n)}$, we can easily assign values to the coefficients in the general PDE of the `LinearPDE` class:

$$\begin{array}{lll} A_{ij} = \kappa \delta_{ij} & D = \omega & Y = f \\ d = \eta & y = g & \end{array} \tag{1.28}$$

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.[6] In this diffusion example we do not need to define a characteristic function q because the boundary conditions we consider in Equation (1.24) are just the natural boundary conditions which are already defined in the `LinearPDE` class (shown in Equation (1.26)).

The Helmholtz equation can be set up the following way[7]:

```
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 an `esys.escript` function returning the Kronecker symbol.

The coefficients can set by several calls to `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()
```

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

$$A_{jl} = A_{lj} \ . \tag{1.29}$$

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` 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])
```

[6] There is a difference in `esys.escript` for a coefficient to be not present and set to zero. Since in the former case the coefficient is not processed, it is more efficient to leave it undefined instead of assigning zero to it.

[7] Note that this is not a complete code. The full source code can be found in "helmholtz.py".

```
print mypde.checkSymmetry() # returns False
mypde.setValue(C=kronecker(mydomain)[0])
print mypde.checkSymmetry() # returns True
```

Unfortunately, calling `checkSymmetry` is very expensive and is only recommended for testing and debugging purposes. 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 $\kappa n_i u_{,i} = \kappa n_0$. Thus 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
from esys.weipa import saveVTK
# 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.vtu", sol=u)
```

To visualize the solution 'x0.vtu' you can use the command

```
mayavi -d x0.vtu -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 1.2. `mydomain.getNormal()` returns the outer normal field on the surface of the domain. The function `Lsup` is 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` to 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.

1.3.4 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 (1.22). 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 is equal to T_{ref}. The `LinearPDE` object `mypde` and the coefficients that do not change over time are set up before the loop 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 (1.16) 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` object of the `esys.escript` module defining locations in the `Domain` `mydomain`. The `length()` function imported from the `esys.escript` module returns the Euclidean norm:

$$\|y\| = \sqrt{y_i y_i} = \texttt{esys.escript.length}(y) \tag{1.30}$$

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
from esys.weipa import saveVTK
#... 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 ...
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()
```

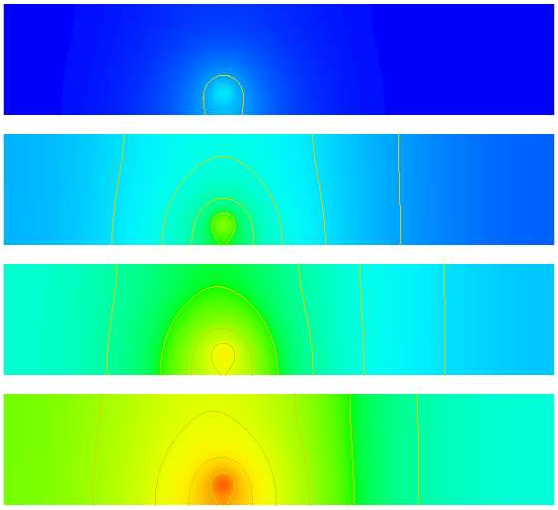


FIGURE 1.6: Results of the Temperature Diffusion Problem for Time Steps 1, 16, 32 and 48

```
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.vtu"%i, temp=T)
```

The script will create the files `T.1.vtu`, `T.2.vtu`, ..., `T.50.vtu` in the directory where the script has been started. The files contain the temperature distributions at time steps $1, 2, i, \ldots, 50$ in the *VTK* file format.

Figure 1.6 shows the result for some selected time steps. An easy way to visualize the results is the command

```
mayavi -d T.1.vtu -m SurfaceMap
```

Use the *Configure Data* window in mayavi to move forward and backward in time.

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

$$\rho u_{i,tt} - \sigma_{ij,j} = 0 \tag{1.31}$$

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

$$\sigma_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i}) \tag{1.32}$$

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

$$\sigma_{ij}n_j = 0 \tag{1.33}$$

for all time $t > 0$.

Here we are modelling a point source at the point x_C in the x_0-direction which is a negative pulse of amplitude U_0 followed by the same positive pulse. In mathematical terms we use

$$u_0(x_C, t) = U_0 \sqrt{2}\frac{(t - t_0)}{\alpha} e^{\frac{1}{2} - \frac{(t-t_0)^2}{\alpha^2}} \tag{1.34}$$

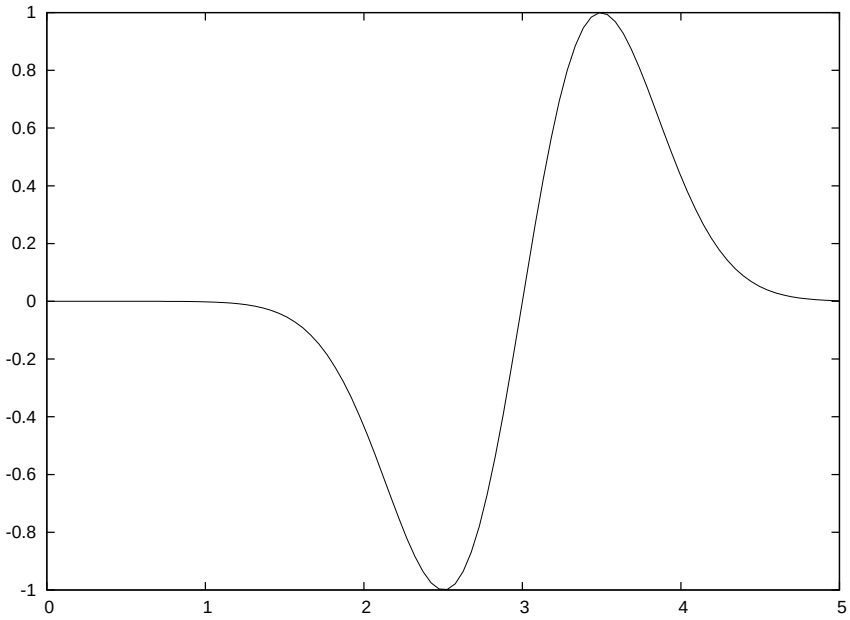


FIGURE 1.7: Input Displacement at Source Point ($\alpha = 0.7$, $t_0 = 3$, $U_0 = 1$).

for all $t \geq 0$ where α is the width of the pulse and t_0 is the time when the pulse changes from negative to positive. In the simulations we will choose $\alpha = 0.3$ and $t_0 = 2$ (see Figure 1.7) and apply the source as a constraint 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

$$u^{(n)} = 2u^{(n-1)} - u^{(n-2)} + h^2 a^{(n)} \tag{1.35}$$

$$\tag{1.36}$$

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

$$u_{,tt} = G(u) \tag{1.37}$$

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

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

$$\rho a_i^{(n)} = \sigma_{ij,j}^{(n-1)} \tag{1.38}$$

and boundary conditions

$$\sigma_{ij}^{(n-1)} n_j = 0 \tag{1.39}$$

derived from Equation (1.33) where

$$\sigma_{ij}^{(n-1)} \quad = \quad \lambda u_{k,k}^{(n-1)} \delta_{ij} + \mu(u_{i,j}^{(n-1)} + u_{j,i}^{(n-1)}). \tag{1.40}$$

We also need to apply the constraint

$$a_0^{(n)}(x_C, t) = U_0 \frac{\sqrt{(2.)}}{\alpha^2}(4\frac{(t-t_0)^3}{\alpha^3} - 6\frac{t-t_0}{\alpha})e^{\frac{1}{2} - \frac{(t-t_0)^2}{\alpha^2}} \tag{1.41}$$

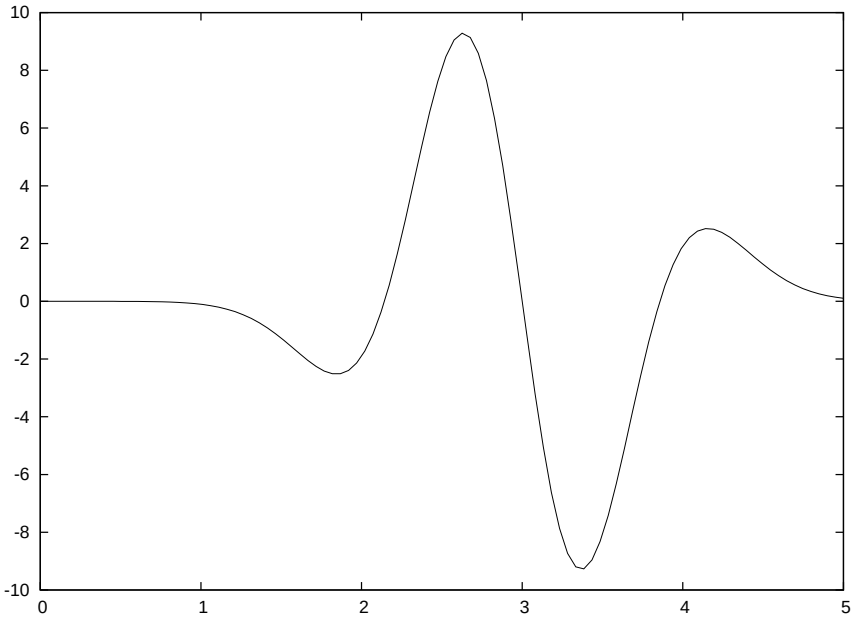


FIGURE 1.8: Input Acceleration at Source Point ($\alpha = 0.7$, $t_0 = 3$, $U_0 = 1$).

which is derived from equation 1.34 by calculating the second order time derivative (see Figure 1.8). Now we have converted our problem for displacement, $u^{(n)}$, into a problem for acceleration, $a^{(n)}$, which 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` package 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

$$D_{ij}a_j^{(n)} = -X_{ij,j} \ . \tag{1.42}$$

The natural boundary condition

$$n_j X_{ij} = 0 \tag{1.43}$$

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

$$D_{ij} = \rho\delta_{ij} \quad X_{ij} = -\sigma_{ij}^{(n-1)} \tag{1.44}$$

Moreover we need to define the location r where the constraint 1.41 is applied. We will apply the constraint on a small sphere of radius R around x_C (we will use 3% of the width of the domain):

$$q_i(x) = \begin{cases} 1 & \text{where } \|x - x_c\| \leq R \\ 0 & \text{otherwise} \end{cases} \tag{1.45}$$

The following script defines 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.

```
def wavePropagation(domain,h,tend,lam,mu,rho, x_c, src_radius, U0):
    # lists to collect displacement at point source which is returned
    # to the caller
    ts, u_pc0, u_pc1, u_pc2 = [], [], [], []
```

```
    x=domain.getX()
    # ... open new PDE ...
    mypde=LinearPDE(domain)
    mypde.getSolverOptions().setSolverMethod(mypde.getSolverOptions().HRZ_LUMPING)
    kronecker=identity(mypde.getDim())
    dunit=numpy.array([1., 0., 0.]) # defines direction of point source
    mypde.setValue(D=kronecker*rho, q=whereNegative(length(x-xc)-src_radius)*dunit)
    # ... set initial values ....
    n=0
    # for first two time steps
    u=Vector(0., Solution(domain))
    u_last=Vector(0., Solution(domain))
    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)
    ts.append(t)
    u_pc0.append(u_pc[0])
    u_pc1.append(u_pc[1])
    u_pc2.append(u_pc[2])

    while t<tend:
      t+=h
      # ... get current stress ....
      g=grad(u)
      stress=lam*trace(g)*kronecker+mu*(g+transpose(g))
      # ... get new acceleration ....
      amplitude=U0*(4*(t-t0)**3/alpha**3-6*(t-t0)/alpha)*sqrt(2.)/alpha**2 \
                                              *exp(1./2.-(t-t0)**2/alpha**2)
      mypde.setValue(X=-stress, r=dunit*amplitude)
      a=mypde.getSolution()
      # ... get new displacement ...
      u_new=2*u-u_last+h**2*a
      # ... shift displacements ....
      u_last=u
      u=u_new
      n+=1
      print(n,"-th time step, t=",t)
      u_pc=L.getValue(u)
      print("u at point charge=",u_pc)
      # save displacements at point source to file for t > 0
      ts.append(t)
      u_pc0.append(u_pc[0])
      u_pc1.append(u_pc[1])
      u_pc2.append(u_pc[2])

      # ... 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), \
                               tensor = stress, Ux = u[0])

    return ts, u_pc0, u_pc1, u_pc2
```

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

The statement

```
mypde.getSolverOptions().setSolverMethod(mypde.getSolverOptions().HRZ_LUMPING)
```

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, see also Section 4.4.

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` (i.e. `transpose(g)[i,j]` $==$ `g[j,i]`).

We initialize the values of `u` and `u_last` to be zero. It is important to initialize both with the solution `FunctionSpace` as they have to be seen as solutions of PDEs from previous time steps. In fact, the `grad` does not accept arguments with a certain `FunctionSpace`, for more details see Section 3.2.3.

The `Locator` class is designed to extract values at a given location (in this case x_C) from functions such as the displacement vector `u`. Typically `Locator` is used in the following way:

```
L=Locator(domain, xc)
u=...
u_pc=L.getValue(u)
```

The return value `u_pc` is the value of `u` at the location `xc`[8]. The values are collected in the lists `u_pc0`, `u_pc1` and `u_pc2` together with the corresponding time marker in `ts`. These values are handed back to the caller. Later we will show ways to access these data.

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 than the stress which is actually present at the current time step. Schemes using this approach are called explicit time integration schemes. The backward Euler scheme we have used in Chapter 1.3 is an example of an implicit scheme. In this case one uses the actual status of each variable at a particular time rather than values from previous time steps. This will lead to a problem which is more expensive to solve, in particular for non-linear cases. Although explicit time integration schemes are cheap to finalize a single time step, they need significantly smaller time steps than implicit schemes and can suffer from stability problems. Therefore they require a very careful selection of the time step size h.

An easy, heuristic way of choosing an appropriate time step size is the CourantFriedrichsLewy condition (CFL condition) which says that within a time step 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

$$h = \frac{1}{5}\sqrt{\frac{\rho}{\lambda+2\mu}}\Delta x \tag{1.46}$$

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, i.e. `l0` and `l1`). The variable `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 depth is chosen such that the elements become cubic. We chose 10 for the number of elements in the x_2-direction so that the computation is 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
U0 = 1. # amplitude of point source
```

[8] In fact, it is the finite element node which is closest to the given position. The usage of `Locator` is MPI safe.

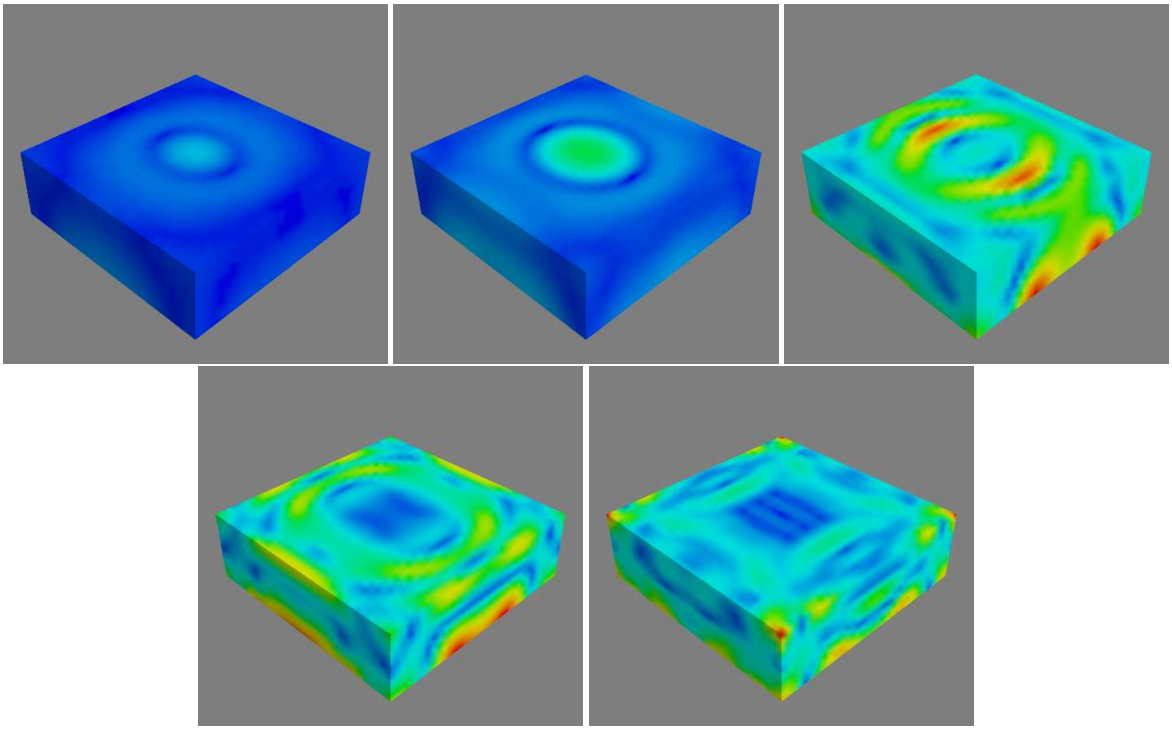


FIGURE 1.9: Selected time steps ($n = 11, 22, 32, 36$) of a wave propagation over a 10km $\times$ 10km $\times$ 3.125km block from a point source initially at (5km, 5km, 0) with time step size $h = 0.02083$. Color represents the displacement. Here the view is oriented onto the bottom face.

```
# spherical source at middle of bottom face
xc=[width/2.,width/2.,0.]
# define small radius around point xc
src_radius = 0.03*width
print("src_radius =",src_radius)
mydomain=Brick(ne, ne, 10, l0=width, l1=width, l2=10.*width/32.)
h=(1./5.)*inf(sqrt(rho/(lam+2*mu)))*inf(domain.getSize())
print("time step size =",h)
ts, u_pc0, u_pc1, u_pc2 =  \
        wavePropagation(mydomain, h, tend, lam, mu, rho, xc, src_radius, U0)
```

The `domain.getSize()` function returns the local element size Δx. Using `inf` ensures that the CFL condition 1.46 holds everywhere in the domain.

The script is available as `wave.py` in the example directory . To visualize the results from the data directory:

```
mayavi2 -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 backward and forward in time, and also to choose the results (acceleration, displacement or u_x) by using *Select Scalar*. Figure 1.9 shows the results for the displacement at various time steps.

It remains to show some possibilities to inspect the collected data `u_pc0`, `u_pc1` and `u_pc2`. One way is to write the data to a file and then use an external package such as *gnuplot*[37], Excel or OpenOffice.org Calc to read the data for further analysis. The following code shows one possible way to write the data to the file `./data/U_pc.csv`:

```
u_pc_data=FileWriter('./data/U_pc.csv')
for i in xrange(len(ts)):
    u_pc_data.write("%f %f %f %f\n"%(ts[i],u_pc0[i],u_pc1[i],u_pc2[i]))
u_pc_data.close()
```

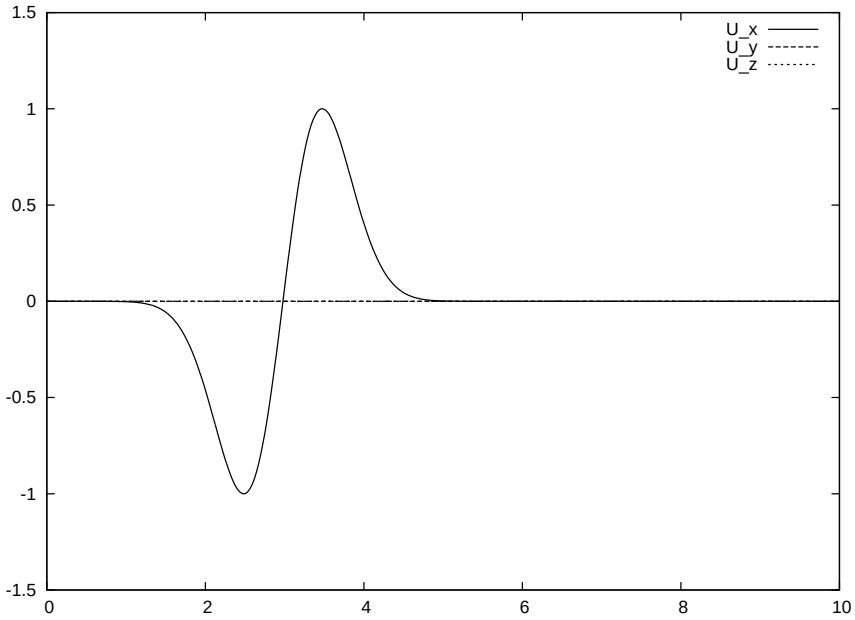


FIGURE 1.10: Amplitude at Point source from the Simulation

The file `U_pc.csv` 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*[37]the command:

```
plot 'U_pc.csv' u 1:2 title 'U_x' w l lw 2, 'U_pc.csv' u 1:3 title 'U_y' w l
lw 2, 'U_pc.csv' u 1:4 title 'U_z' w l lw 2
```

will reproduce Figure 1.10 (As expected this is identical to the input signal shown in Figure 1.7). It is pointed out that we are not using the standard *python* `open` to write to the file `U_pc.csv` as it is not safe when running `esys.escript` under MPI, see Chapter 2 for more details.

Alternatively, one can implement plotting the results at run time rather than in a post-processing step. This avoids the generation of an intermediate data file. In *escript* the preferred way of creating 2D plots of time dependent data is `matplotlib`. The following script creates the plot and writes it into the file `u_pc.png` in the PNG image format:

```
import matplotlib.pyplot as plt
if getMPIRankWorld() == 0:
    plt.title("Displacement at Point Source")
    plt.plot(ts, u_pc0, '-', label="x_0", linewidth=1)
    plt.plot(ts, u_pc1, '-', label="x_1", linewidth=1)
    plt.plot(ts, u_pc2, '-', label="x_2", linewidth=1)
    plt.xlabel('time')
    plt.ylabel('displacement')
    plt.legend()
    plt.savefig('u_pc.png', format='png')
```

You can add `plt.show()` to create an interactive browser window. Notice that by checking the condition `getMPIRankWorld()==0` the plot is generated on one processor only (in this case the rank 0 processor) when run under *MPI*.

Both options for processing the point source data are include in the example file `wave.py`. There are other options available to process these data in particular through the *SciPy*[6] package, e.g. Fourier transformations. It

is beyond the scope of this user's guide to document the usage of *SciPy*[6] for time series analysis but it is highly recommended that users use *SciPy*[6] for any further data processing.

1.4 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:

$$-\sigma_{ij,j} = 0 \tag{1.47}$$

where the stress σ is given by

$$\sigma_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i}) - (\lambda + \frac{2}{3}\mu)\ \alpha\ (T - T_{ref})\delta_{ij}\ . \tag{1.48}$$

In this formula λ and μ are the Lame coefficients, α is the temperature expansion coefficient, T is the temperature distribution and T_{ref} a reference temperature. Note that Equation (1.47) is similar to Equation (1.31) introduced in Section **??** but the inertia term $\rho u_{i,tt}$ has been dropped as we assume a static scenario here. Moreover, in comparison to the Equation (1.32) definition of stress σ in Equation (1.48) an extra term is introduced to bring in stress due to volume changes through temperature dependent expansion.

Our domain is the unit cube

$$\Omega = \{(x_i)|0 \le x_i \le 1\} \tag{1.49}$$

On the boundary the normal stress component is set to zero

$$\sigma_{ij}n_j = 0 \tag{1.50}$$

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

$$u_i(x) = 0 \quad \text{where} \quad x_i = 0 \tag{1.51}$$

For the temperature distribution we use

$$T(x) = T_0 e^{-\beta\|x-x^c\|} \tag{1.52}$$

with a given positive constant β and location x^c in the domain.

When we insert Equation (1.48) 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. For a system of PDEs and a solution with several components the `LinearPDE` class takes PDEs of the form

$$-(A_{ijkl}u_{k,l})_{,j} = -X_{ij,j}\ . \tag{1.53}$$

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

$$n_j A_{ijkl} u_{k,l} = n_j X_{ij} \tag{1.54}$$

while constraints take the form

$$u_i = r_i \text{ where } q_i > 0 \tag{1.55}$$

r and q are each a rank-1 `Data` object. We can easily identify the coefficients in Equation (1.53):

$$A_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{1.56}$$

$$X_{ij} = (\lambda + \frac{2}{3}\mu)\ \alpha\ (T - T_{ref})\delta_{ij} \tag{1.57}$$

$$\tag{1.58}$$

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

$$q_i(x) = \begin{cases} 1 & x_i = 0 \\ 0 & \text{otherwise} \end{cases} \tag{1.59}$$

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 (1.48) to zero.

Analogously to the concept of symmetry for a single PDE, we call the PDE defined by Equation (1.53) symmetric if

$$A_{ijkl} = A_{klij} \tag{1.60}$$

(1.61)

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

$$\sigma_{mises} = \sqrt{\frac{1}{2}((\sigma_{00}-\sigma_{11})^2 + (\sigma_{11}-\sigma_{22})^2 + (\sigma_{22}-\sigma_{00})^2) + 3(\sigma_{01}^2 + \sigma_{12}^2 + \sigma_{20}^2)} \tag{1.62}$$

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

The following script, which is available in `heatedblock.py` in the example directory, solves the Lame equation and writes the displacements and the von-Mises stress into a file `deform.vtu` in the *VTK* file format:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Brick
from esys.weipa import saveVTK
#... 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-Mises stress
g=grad(u)
sigma=mu*(g+transpose(g))+lam*trace(g)*kronecker(mydomain)-sigma0
sigma_mises=sqrt(((sigma[0,0]-sigma[1,1])**2+(sigma[1,1]-sigma[2,2])**2+ \
                  (sigma[2,2]-sigma[0,0])**2)/2. \
```

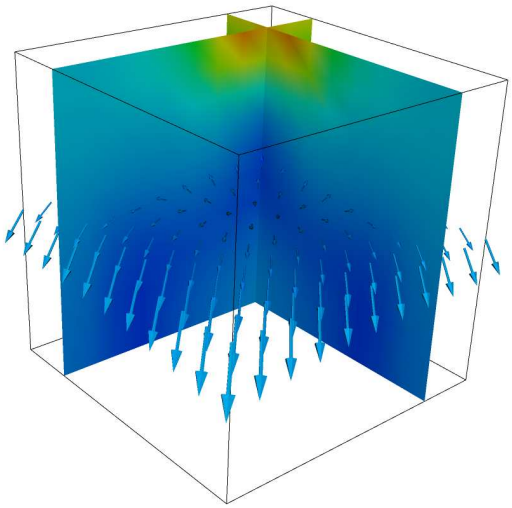


FIGURE 1.11: von-Mises Stress and Displacement Vectors

```
                    +3*(sigma[0,1]**2 + sigma[1,2]**2 + sigma[2,0]**2))
#... output ...
saveVTK("deform.vtu", disp=u, stress=sigma_mises)
```

Finally, the results can be visualized by calling

```
mayavi2 -d deform.vtu -f CellToPointData -m VelocityVector -m SurfaceMap
```

Note that the filter CellToPointData is applied to create a smoother representation of the von-Mises stress. Figure 1.11 shows the results where the colour of the vertical planes represent the von-Mises stress and a horizontal plane of arrows shows the displacements vectors.

1.5 Stokes Flow

In this section we will look at Computational Fluid Dynamics (CFD) to simulate the flow of fluid under the influence of gravity. The `StokesProblemCartesian` class will be used to calculate the velocity and pressure of the fluid. The fluid dynamics is governed by the Stokes equation. In geophysical problems the velocity of fluids is 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:

$$\nabla \cdot (\eta(\nabla \vec{v} + \nabla^T \vec{v})) - \nabla p = -f, \tag{1.63}$$

with the incompressibility condition

$$\nabla \cdot \vec{v} = 0. \tag{1.64}$$

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):

$$-(\eta(v_{i,j} + v_{j,i}))_{,j} - p_{,i} = f_i, \tag{1.65}$$

with the incompressibility condition

$$-v_{i,i} = 0. \tag{1.66}$$

The subscript comma i denotes the derivative of the function with respect to x_i. The body force f in Equation (1.65) is the gravity acting in the x_3 direction and is given as $f = -g\rho\delta_{i3}$. The Stokes equation is a saddle point problem, and can be solved using a Uzawa scheme. A class called `StokesProblemCartesian` in `esys.escript`

can be used to solve for velocity and pressure. A more detailed discussion of the class can be found in Chapter 6. In order to keep numerical stability and satisfy the CourantFriedrichsLewy condition (CFL condition) , the time-step size needs to be kept below a certain value. The Courant number is defined as:

$$C = \frac{v\delta t}{h} \tag{1.67}$$

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 time-step size was calculated for a Courant number of 0.4.

The following *python* script is the setup for the Stokes flow simulation, and is available in the example directory as `fluid.py`. It starts off by importing the classes, such as the `StokesProblemCartesian` class, for solving the Stokes equation and the incompressibility condition for velocity and pressure. Physical constants are defined for the viscosity and density of the fluid, along with the acceleration due to gravity. Solver settings are set for the maximum iterations and tolerance; the default solver used is PCG. The mesh is defined as a rectangle, to represent the body of fluid. We are using 20×20 elements with piecewise linear elements for the pressure and for velocity but the elements are subdivided for the velocity. This approach is called *macro elements* and needs to be applied to make sure that the discretized problem has a unique solution, see [12] for details[9]. The fact that pressure and velocity are represented in different ways is expressed by

```
velocity=Vector(0., Solution(mesh))
pressure=Scalar(0., ReducedSolution(mesh))
```

The gravitational force is calculated based on the fluid density and the acceleration due to gravity. The boundary conditions are set for a slip condition at the base and the left face of the domain. At the base fluid movement in the x_0-direction is free, but fixed in the x_1-direction, and similarly at the left face fluid movement in the x_1-direction is free but fixed in the x_0-direction. An instance of the `StokesProblemCartesian` class is defined for the given computational mesh, and the solver tolerance set. Inside the `while` loop, the boundary conditions, viscosity and body force are initialized. The Stokes equation is then solved for velocity and pressure. The time-step size is calculated based on the CourantFriedrichsLewy condition (CFL condition) , to ensure stable solutions. The nodes in the mesh are then displaced based on the current velocity and time-step size, to move the body of fluid. The output for the simulation of velocity and pressure is then saved to a file for visualization.

```
from esys.escript import *
import esys.finley
from esys.escript.linearPDEs import LinearPDE
from esys.escript.models import StokesProblemCartesian
from esys.weipa import saveVTK

# physical constants
eta=1.
rho=100.
g=10.

# solver settings
tolerance=1.0e-4
max_iter=200
t_end=50
t=0.0
time=0
verbose=True

# define mesh
H=2.
L=1.
W=1.
mesh = esys.finley.Rectangle(l0=L, l1=H, order=-1, n0=20, n1=20)
coordinates = mesh.getX()
```

[9] Alternatively, one can use second order elements for the velocity and first order elements for pressure on the same element. You can set `order=2` in `esys.finley.Rectangle`.

```
# gravitational force
Y=Vector(0., Function(mesh))
Y[1] = -rho*g

# element spacing
h = Lsup(mesh.getSize())

# boundary conditions for slip at base
boundary_cond=whereZero(coordinates[1])*[0.0,1.0]+whereZero(coordinates[0])*[1.0,0.0]

# velocity and pressure vectors
velocity=Vector(0., Solution(mesh))
pressure=Scalar(0., ReducedSolution(mesh))

# Stokes Cartesian
solution=StokesProblemCartesian(mesh)
solution.setTolerance(tolerance)

while t <= t_end:
  print(" ----- Time step = %s -----"%t)
  print("Time = %s seconds"%time)

  solution.initialize(fixed_u_mask=boundary_cond, eta=eta, f=Y)
  velocity,pressure=solution.solve(velocity,pressure,max_iter=max_iter, \
                                   verbose=verbose)

  print("Max velocity =", Lsup(velocity), "m/s")

  # CFL condition
  dt=0.4*h/(Lsup(velocity))
  print("dt =", dt)

  # displace the mesh
  displacement = velocity * dt
  coordinates = mesh.getX()
  mesh.setX(coordinates + displacement)

  time += dt

  vel_mag = length(velocity)

  #save velocity and pressure output
  saveVTK("vel.%2.2i.vtu"%t, vel=vel_mag, vec=velocity, pressure=pressure)
  t = t+1.
```

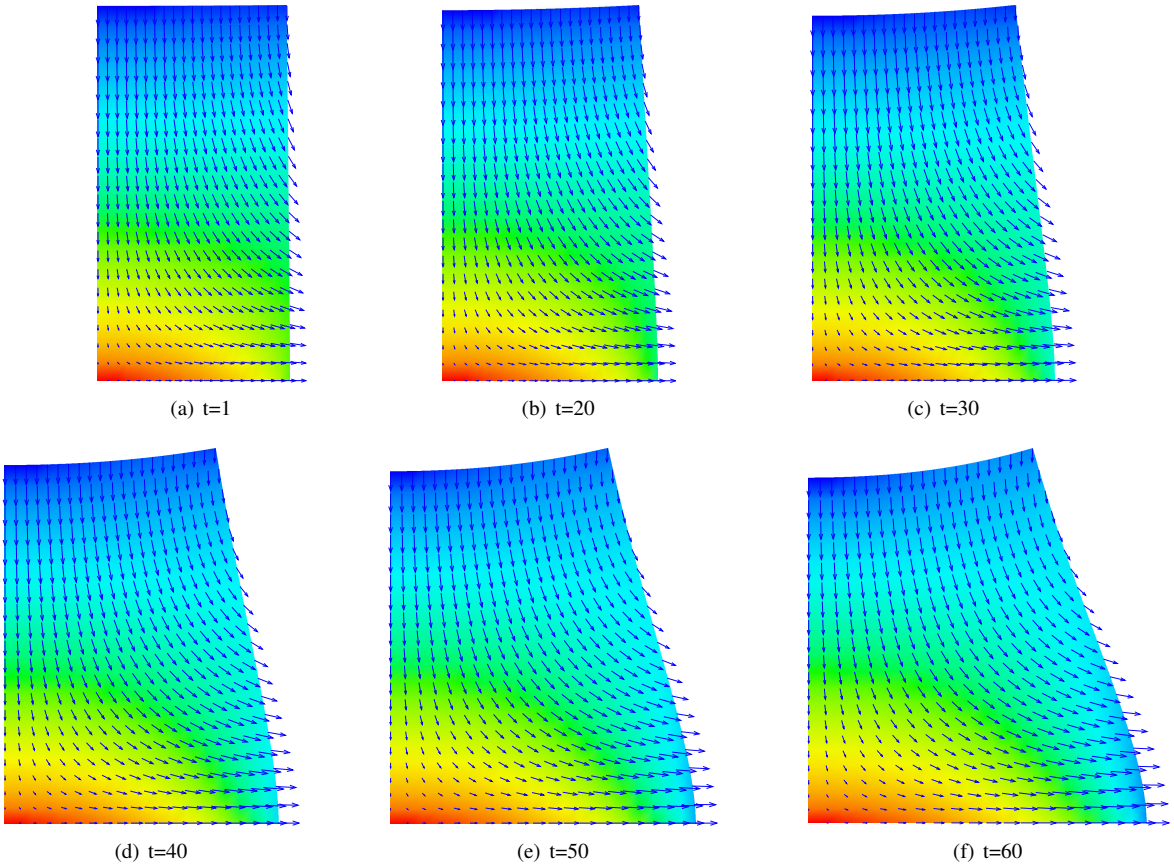
The results from the simulation can be viewed with *mayavi*, by executing the following command:

```
mayavi2 -d vel.00.vtu -m SurfaceMap
```

Colour-coded scalar maps and velocity flow fields can be viewed by selecting them in the menu. The time-steps can be swept through to view a movie of the simulation. Figure 1.12 shows the simulation output. Velocity vectors and a colour map for pressure are shown. As the time progresses the body of fluid falls under the influence of gravity. The view used here to track the fluid is the Lagrangian view, since the mesh moves with the fluid. One of the disadvantages of using the Lagrangian view is that the elements in the mesh become severely distorted after a period of time and introduce solver errors. To get around this limitation the Level Set Method can be used, with the Eulerian point of view for a fixed mesh.

1.6 Slip on a Fault

In this example we illustrate how to calculate the stress distribution around a fault in the Earth's crust caused by a slip through an earthquake.



(a) t=1 (b) t=20 (c) t=30

(d) t=40 (e) t=50 (f) t=60

FIGURE 1.12: Simulation output for Stokes flow. Fluid body starts off as a rectangular shape, then progresses downwards under the influence of gravity. Colour coded distribution represents the scalar values for pressure. Velocity vectors are displayed at each node in the mesh to show the flow field. Computational mesh used was 20×20 elements.

To simplify the presentation we assume a simple domain $\Omega = [0,1]^2$ with a vertical fault in its center as illustrated in Figure 1.13. We assume that the slip distribution s_i on the fault is known. We want to calculate the distribution of the displacements u_i and stress σ_{ij} in the domain. Further, we assume an isotropic, linear elastic material model of the form

$$\sigma_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i}) \tag{1.68}$$

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

$$\sigma_{ij}n_j = 0 \tag{1.69}$$

and normal displacements are set to zero:

$$u_i n_i = 0 \tag{1.70}$$

The stress needs to fulfill the momentum equation

$$-\sigma_{ij,j} = 0 \tag{1.71}$$

This problem is very similar to the elastic deformation problem presented in Section 1.4. However, we need to address an additional challenge: the displacement u_i is in fact discontinuous across the fault, but we are in the lucky situation that we know the jump of the displacements across the fault. This is in fact the given slip s_i. So we can split the total distribution u_i into a component v_i which is continuous across the fault and the known slip s_i

$$u_i = v_i + \frac{1}{2}s_i^{\pm} \tag{1.72}$$

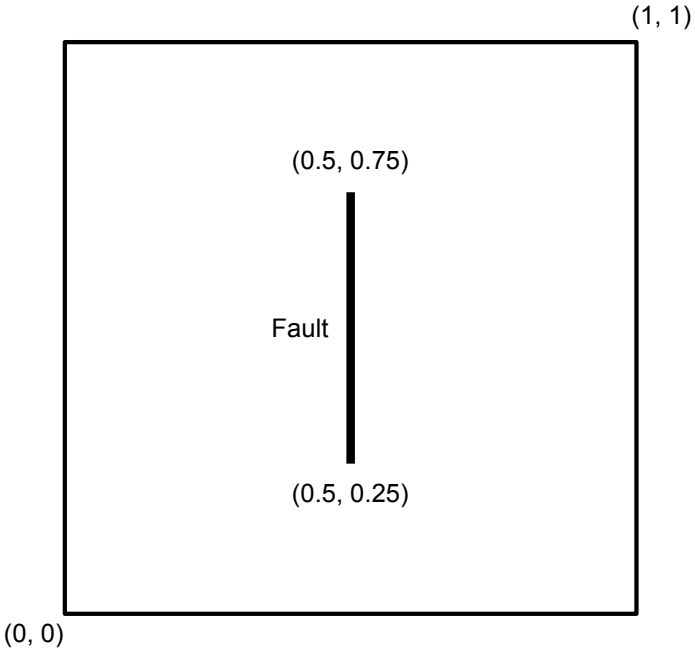


FIGURE 1.13: Domain $\Omega = [0, 1]^2$ with a vertical fault of length 0.5.

where $s^{\pm} = s$ when right of the fault and $s^{\pm} = -s$ when left of the fault. We assume that $s^{\pm} = 0$ when sufficiently away from the fault.

We insert this into the stress definition in Equation (1.68)

$$\sigma_{ij} = \sigma^c_{ij} + \frac{1}{2}\sigma^s_{ij} \tag{1.73}$$

with

$$\sigma^c_{ij} = \lambda v_{k,k}\delta_{ij} + \mu(v_{i,j} + v_{j,i}) \tag{1.74}$$

and

$$\sigma^s_{ij} = \lambda s^{\pm}_{k,k}\delta_{ij} + \mu(s^{\pm}_{i,j} + s^{\pm}_{j,i}). \tag{1.75}$$

In fact, σ^s_{ij} defines a stress jump across the fault. An easy way to construct this function is to use a function χ which is 1 on the right and -1 on the left side from the fault. One can then set

$$\sigma^s_{ij} = \chi \cdot (\lambda s_{k,k}\delta_{ij} + \mu(s_{i,j} + s_{j,i})) \tag{1.76}$$

assuming that s is extended by zero away from the fault. After inserting Equation (1.73) into (1.71) we get the differential equation

$$-\sigma^c_{ij,j} = \frac{1}{2}\sigma^s_{ij,j} \tag{1.77}$$

Together with the definition (1.74) we have a differential equation for the continuous function v_i. Notice that the boundary condition (1.70) and (1.69) transfer to v_i and σ^c_{ij} as s is zero away from the fault. In Section 1.4 we have discussed how this problem is solved using the `LinearPDE` class. We refer to this section for further details.

To define the fault we use the `FaultSystem` class introduced in Section 6.4. The following statements define a fault system `fs` and add the fault `1` to the system:

```
fs=FaultSystem(dim=2)
fs.addFault(fs.addFault(V0=[0.5,0.25], strikes=90*DEG, ls=0.5, tag=1)
```

The fault added starts at point $(0.5, 0.25)$ has length 0.5 and points north. The main purpose of the `FaultSystem` class is to define a parameterization of the fault using a local coordinate system. One can inquire the class to get the range used to parameterize a fault.

```
p0,p1 = fs.getW0Range(tag=1)
```

Typically `p0` is equal to zero while `p1` is equal to the length of the fault. The parameterization is given as a mapping from a set of local coordinates onto a parameter range (in our case the range `p0` to `p1`). For instance, to map the entire domain `mydomain` onto the fault one can use

```
x = mydomain.getX()
p,m = fs.getParametrization(x, tag=1)
```

Of course there is the problem that not all locations are on the fault. For those locations which are on the fault `m` is set to 1, otherwise 0 is used. So on return the values of `p` define the value of the fault parameterization (typically the distance from the starting point of the fault along the fault) where `m` is positive. On all other locations the value of `p` is undefined. Now `p` can be used to define a slip distribution on the fault via

```
s = m*(p-p0)*(p1-p)/((p1-p0)/2)**2*slip_max*[0.,1.]
```

Notice the factor `m` which ensures that `s` is zero away from the fault. It is important that the slip is zero at the ends of the faults.

We can now put all components together to get the script:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.escript.models import FaultSystem
from esys.finley import Rectangle
from esys.weipa import saveVTK
from esys.escript.unitsSI import DEG

#... set some parameters ...
lam=1.
mu=1
slip_max=1.
mydomain = Rectangle(l0=1.,l1=1.,n0=16, n1=16)  # n1 needs to be a multiple of 4!
# .. create the fault system
fs=FaultSystem(dim=2)
fs.addFault(V0=[0.5,0.25], strikes=90*DEG, ls=0.5, tag=1)
# ... create a slip distribution on the fault
p, m=fs.getParametrization(mydomain.getX(), tag=1)
p0,p1= fs.getW0Range(tag=1)
s=m*(p-p0)*(p1-p)/((p1-p0)/2)**2*slip_max*[0.,1.]
# ... calculate stress according to slip:
D=symmetric(grad(s))
chi, d=fs.getSideAndDistance(D.getFunctionSpace().getX(), tag=1)
sigma_s=(mu*D+lam*trace(D)*kronecker(mydomain))*chi
#... 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
# ... fix displacement in normal direction
x=mydomain.getX()
msk=whereZero(x[0])*[1.,0.] + whereZero(x[0]-1.)*[1.,0.] \
   +whereZero(x[1])*[0.,1.] + whereZero(x[1]-1.)*[0.,1.]
mypde.setValue(A=C, X=-0.5*sigma_s, q=msk)
#... solve pde ...
mypde.getSolverOptions().setVerbosityOn()
v=mypde.getSolution()
# .. write the displacement to file:
D=symmetric(grad(v))
```

```
sigma=(mu*D+lam*trace(D)*kronecker(mydomain))+0.5*sigma_s
saveVTK("slip.vtu", disp=v+0.5*chi*s, stress=sigma)
```

The script creates the file `slip.vtu` which contains the total displacements and stress. These values are stored as cell-centered data. See Figure 1.14 for a visualization of the result.

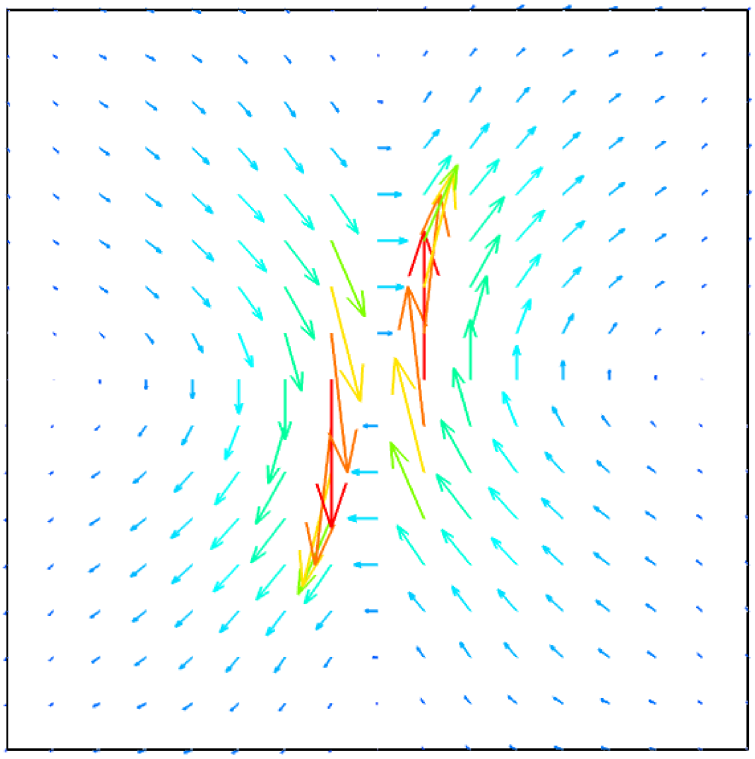


FIGURE 1.14: Total Displacement after the slip event

CHAPTER
TWO

Execution of an *escript* Script

2.1 Overview

A typical way of starting your *escript* script `myscript.py` is with the **`run-escript`** command[1]. This command was renamed from **`escript`** (used in previous releases) to avoid clashing with an unrelated program installed by default on some systems. Most 3.1 releases[2] of `esys.escript` allow either **`run-escript`** or **`escript`** to be used but the latter name will be removed in future releases. To run your script, issue[3]

```
run-escript myscript.py
```

as already shown in Section 1.2. In some cases it can be useful to work interactively, e.g. when debugging a script, with the command

```
run-escript -i myscript.py
```

This will execute `myscript.py` and when it completes (or an error occurs), a *python* prompt will be provided. To leave the prompt press `Control-d` (`Control-z` on *MS Windows*).

To run the script using four threads (e.g. if you have a multi-core processor) you can use

```
run-escript -t 4 myscript.py
```

This requires *escript* to be compiled with *OpenMP* [24] support. To run the script using *MPI* [19] with 8 processes use

```
run-escript -p 8 myscript.py
```

If the processors which are used are multi-core processors or you are working on a multi-processor shared memory architecture you can use threading in addition to *MPI*. For instance to run 8 *MPI* processes with 4 threads each, use the command

```
run-escript -p 8 -t 4 myscript.py
```

In the case of a supercomputer or a cluster, you may wish to distribute the workload over a number of nodes[4]. For example, to use 8 nodes with 4 *MPI* processes per node, write

```
run-escript -n 8 -p 4 myscript.py
```

Since threading has some performance advantages over processes, you may specify a number of threads as well:

```
run-escript -n 8 -p 4 -t 2 myscript.py
```

This runs the script on 8 nodes, with 4 processes per node and 2 threads per process.

[1] The **`run-escript`** launcher is not supported under *MS Windows* yet.
[2] i.e. not *MS Windows* or Ubuntu 9.10
[3] For this discussion, it is assumed that **`run-escript`** is included in your **PATH** environment. See the installation guide for details.
[4] For simplicity, we will use the term *node* to refer to either a node in a supercomputer or an individual machine in a cluster

2.2 Options

The general form of the **run-escript** launcher is as follows:

run-escript [-n nn] [-p np] [-t nt] [-f hostfile] [-x] [-V] [-e] [-h] [-v] [-o] [-c] [-i] [-b] [file] [ARGS]

where file is the name of a script and ARGS are the arguments to be passed to the script. The **run-escript** program will import your current environment variables. If no file is given, then you will be presented with a regular *python* prompt (see -i for restrictions).

The options have the following meaning:

-n nn the number of compute nodes nn to be used. The total number of process being used is $nn \cdot ns$. This option overwrites the value of the **ESCRIPT_NUM_NODES** environment variable. If a hostfile is given (see below), the number of nodes needs to match the number of hosts given in that file. If $nn > 1$ but *escript* is not compiled for *MPI*, a warning is printed but execution is continued with $nn = 1$. If -n is not set the number of hosts in the host file is used. The default value is 1.

-p np the number of *MPI* processes per node. The total number of processes to be used is $nn \cdot np$. This option overwrites the value of the **ESCRIPT_NUM_PROCS** environment variable. If $np > 1$ but *escript* is not compiled for *MPI*, a warning is printed but execution is continued with $np = 1$. The default value is 1.

-t nt the number of threads used per process. The option overwrites the value of the **ESCRIPT_NUM_THREADS** environment variable. If $nt > 1$ but *escript* is not compiled for *OpenMP* , a warning is printed but execution is continued with $nt = 1$. The default value is 1.

-f hostfile the name of a file with a list of host names. Some systems require to specify the addresses or names of the compute nodes where *MPI* processes should be spawned. These addresses or names of the compute nodes are listed in the file with the name hostfile. If -n is set, the number of different hosts defined in hostfile must be equal to the number of requested compute nodes nn. The option overwrites the value of the **ESCRIPT_HOSTFILE** environment variable. By default no host file is used.

-c prints information about the settings used to compile *escript* and stops execution.

-V prints the version of *escript* and stops execution.

-h prints a help message and stops execution.

-i executes the script file and switches to interactive mode after the execution is finished or an exception has occurred. This option is useful for debugging a script. The option cannot be used if more than one process ($nn \cdot np > 1$) is used.

-b do not invoke python. This is used to run non-python programs within an environment set for *escript*.

-e shows additional environment variables and commands used to set up the *escript* environment. This option is useful if users wish to execute scripts without using the **run-escript** command.

-o enables the redirection of messages printed by processors with *MPI* rank greater than zero to the files stdout_r.out and stderr_r.out where r is the rank of the processor. The option overwrites the value of the **ESCRIPT_STDFILES** environment variable.

-v prints some diagnostic information.

2.2.1 Notes

- Make sure that **mpiexec** is in your **PATH** if applicable.
- For MPICH and INTELMPI and for the case a hostfile is present **run-escript** will start the **mpd** daemon before execution.

2.3 Input and Output

When *MPI* is used on more than one process (`nn` $\cdot$ `np` > 1) no input from the standard input is accepted. Standard output on any process other than the master process (`rank` =0) will also not be available. Error output from any processor will be redirected to the node where **`run-escript`** has been invoked. If the -o Option or **ESCRIPT_STDFILES** is set[5], then the standard and error output from any process other than the master process will be written to files of the names `stdout_r.out` and `stderr_r.out` (where `r` is the rank of the process).

If files are created or read by individual *MPI* processes with information local to the process (e.g. in the `dump` function) and more than one process is used (`nn` $\cdot$ `np` > 1), the *MPI* process rank is appended to the file names. This is to avoid problems if processes are using a shared file system. Files which collect data that are global for all *MPI* processors are created by the process with *MPI* rank 0 only. Users should keep in mind that if the file system is not shared among the processes, then a file containing global information which is read by all processors needs to be copied to the local file system(s) before **`run-escript`** is invoked.

2.4 Hints for MPI Programming

In general a script based on the `esys.escript` module does not require modifications to run under *MPI*. However, one needs to be careful if other modules are used.

When *MPI* is used on more than one process (`nn`$\cdot$`np` > 1) the user needs to keep in mind that several copies of his script are executed at the same time[6] while data exchange is performed through the `esys.escript` module.

This has three main implications:

1. most arguments (`Data` excluded) should have the same values on all processors, e.g. `int`, `float`, `str` and `numpy` parameters.

2. the same operations will be called on all processors.

3. different processors may store different amounts of information.

With a few exceptions[7], values of types `int`, `float`, `str` and `numpy` returned by `esys.escript` will have the same value on all processors. If values produced by other modules are used as arguments, the user has to make sure that the argument values are identical on all processors. For instance, the usage of a random number generator to create argument values bears the risk that the value may depend on the processor.

Some operations in `esys.escript` require communication with all processors executing the job. It is not always obvious which operations these are. For example, `Lsup` returns the largest value on all processors. `getValue` on `Locator` may refer to a value stored on another processor. For this reason it is better if scripts do not have conditional operations (which manipulate data) based on which processor the script is on. Crashing or hanging scripts can be an indication that this has happened.

It is not always possible to divide data evenly amongst processors. In fact some processors might not have any data at all. Try to avoid writing scripts which iterate over data points, instead try to describe the operation you wish to perform as a whole.

Special attention is required when using files on more than one processor as several processors access the file at the same time. Opening a file for reading is safe, however the user has to make sure that the variables which are set from reading data from files are identical on all processors.

When writing data to a file it is important that only one processor is writing to the file at any time. As all values in `esys.escript` are global it is sufficient to write values on the processor with *MPI* rank 0 only. The `FileWriter` class provides a convenient way to write global data to a simple file. The following script writes to the file `test.txt` on the processor with rank 0 only:

```
from esys.escript import FileWriter
f = FileWriter('test.txt')
f.write('test message')
f.close()
```

[5] That is, it has a non-empty value.
[6] In the case of *OpenMP* only one copy is running but *escript* temporarily spawns threads.
[7] `getTupleForDataPoint`

We strongly recommend using this class rather than *python*'s built-in `open` function as it will guarantee a script which will run in single processor mode as well as under *MPI*.

If the situation occurs that one of the processors throws an exception, for instance when opening a file for writing fails, the other processors are not automatically made aware of this since *MPI* does not handle exceptions. However, *MPI* will still terminate the other processes but may not inform the user of the reason in an obvious way. The user needs to inspect the error output files to identify the exception.

2.5 Lazy Evaluation

Escript now supports lazy evaluation [10]. Lazy evaluation is when expressions are not evaluated until they are actually needed. When applied to suitable problems, it can reduce both the memory and CPU time required to perform a simulation. This implementation is designed to be as transparent as possible; so significant alterations to scripts are not required.

How to use it

To have lazy evaluation applied automatically, put the following command in your script after the imports.

```
from esys.escript import setEscriptParamInt
setEscriptParamInt('AUTOLAZY', 1)
```

To get greater benefit, some fine tuning may be required. If your simulation involves iterating for a number of time steps, you will probably have some state variables which are updated in each iteration based on their value in the previous iteration. For example,

```
x=f(x_previous)
y=g(x)
z=h(y, x, ...)
```

could be modified to:

```
x=f(x_previous)
resolve(x)
y=g(x)
z=h(y, x, ...)
```

The `resolve` command forces x to be evaluated immediately.

When to use it

We believe that problems involving large domains and complicated expressions will benefit most from lazy evaluation. In cases where lazy does provide a benefit, larger domains should give a greater benefit. If you are uncertain, try running a test on a smaller domain first.

CHAPTER
THREE

The `esys.escript` Module

3.1 Concepts

`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`.

3.1.1 Function spaces

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 commonly used:

- `Solution(mydomain)`: solutions of a PDE
- `ReducedSolution(mydomain)`: solutions of a PDE with a reduced smoothness requirement, e.g. using a lower order approximation on the same element or using macro elements
- `ContinuousFunction(mydomain)`: continuous functions, e.g. a temperature distribution
- `Function(mydomain)`: general functions which are not necessarily continuous, e.g. a stress field
- `FunctionOnBoundary(mydomain)`: functions on the boundary of the domain, e.g. a surface pressure
- `FunctionOnContact0(mydomain)`: functions on side 0 of the discontinuity
- `FunctionOnContact1(mydomain)`: functions on side 1 of the discontinuity

In some cases under-integration is used. For these cases the user may use a `FunctionSpace` from the following list:

- `ReducedFunction(mydomain)`
- `ReducedFunctionOnBoundary(mydomain)`

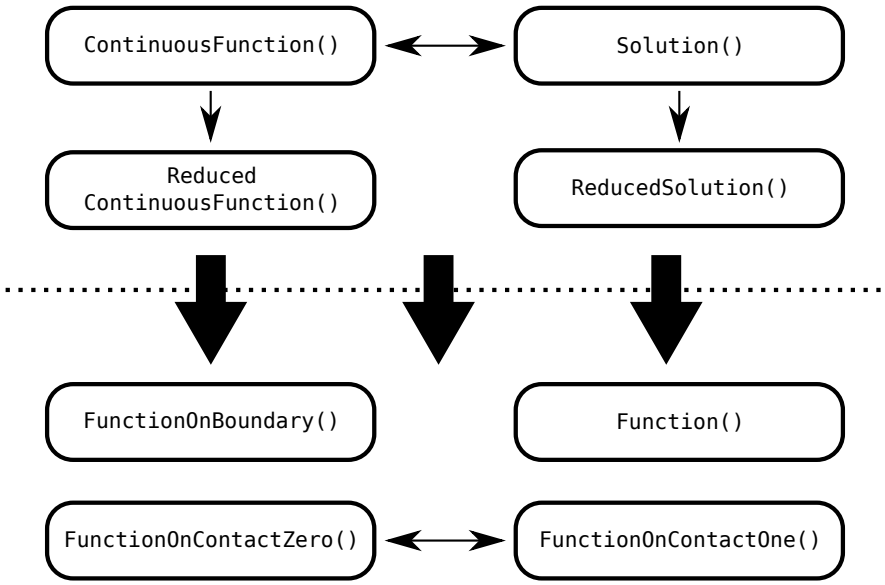


FIGURE 3.1: Dependency of function spaces in `esys.finley`. An arrow indicates that a function in the `FunctionSpace` at the starting point can be interpolated to the `FunctionSpace` of the arrow target. All function spaces above the dotted line can be interpolated to any of the function spaces below the line. See also Section 4.2.

- `ReducedFunctionOnContact0(mydomain)`
- `ReducedFunctionOnContact1(mydomain)`

In comparison to the corresponding full version they use a reduced number of integration nodes (typically one only) to represent values.

The reduced smoothness for a PDE solution is often used to fulfill the Ladyzhenskaya-Babuska-Brezzi condition [12] when solving saddle point problems, e.g. the Stokes equation. A discontinuity is a region within the domain across which functions may be discontinuous. The location of a discontinuity is defined in the `Domain` object. Figure 3.1 shows the dependency between the types of function spaces in `esys.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 a 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, for example 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.

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 nodes 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. The user needs to be aware that an interpolation is not always possible, see Figure 3.1 for `esys.finley`. An alternative approach to change the representation (=`FunctionSpace`) is projection, see Section 4.2.

3.1.2 `Data` Objects

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 `numpy` array or any object, such as a list of floating point numbers, that can be converted into a `numpy.ndarray` [5]. The following two statements create objects which are equivalent to `mydat`:

```
mydat1=Data(value=numpy.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 `numpy.ones((2,3))` which generates a 2×3 matrix as an instance of `numpy.ndarray` filled with ones. The shape of the created `Data` object is taken from the shape of the array. In the second case, the creator converts the initial value, which is a list of lists, into a `numpy.ndarray` 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))` equals `Data(0, Function(myDomain), (d,d))`, e.g. a stress field
- `Tensor4(0,Function(mydomain))` equals `Data(0,Function(myDomain), (d,d,d,d))`, e.g. a Hook tensor field

Here the initial value is 0 but any object that can be converted into a `numpy.ndarray` 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 (e.g. cos, sin, log), and they can be combined point-wise by applying arithmetic operations (e.g. +, - ,* , /). We emphasize 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 operations 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
```

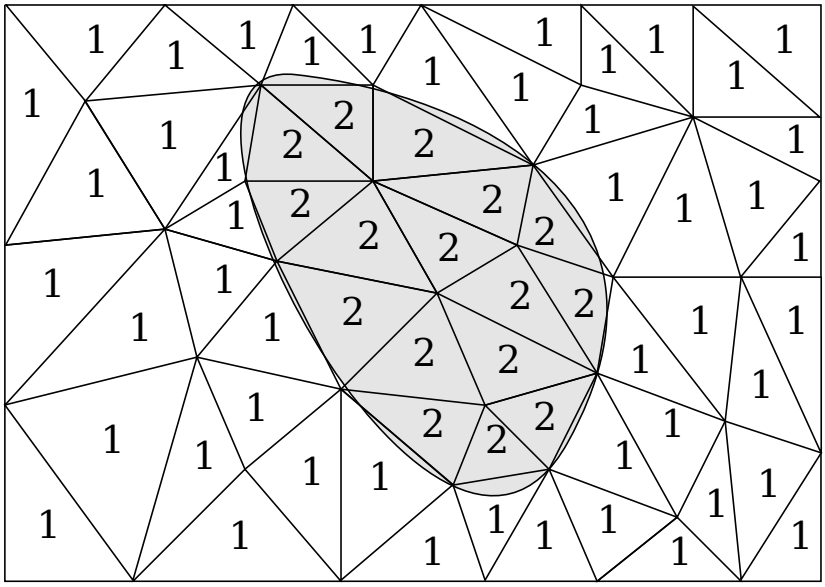


FIGURE 3.2: Element Tagging. A rectangular mesh over a region with two rock types *white* and *gray* is shown. The number in each cell refers to the major rock type present in the cell (1 for *white* and 2 for *gray*).

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`. The result `g` as well as the returned stress will be in the general `FunctionSpace`. 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` but with `g` the function `trace(g)` is in the general `FunctionSpace`. 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 into an appropriate function space according to Figure 3.1. In this example that means `esys.escript` sees `lam` as a function of the general `FunctionSpace`. In 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.

3.1.3 Tagged, Expanded and Constant Data

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 predominantly 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 to use tagged values for `lam` as shown in Figure 3.2 for the stress calculation discussed above:

```
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 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 for models 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 while 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 specifying `expanded=True` in the `Data` object constructor, while tagged data requires calling 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.

3.1.4 Saving and Restoring Simulation Data

`Data` objects can be written to disk files with the `dump` method and read back using the `load` method, both of which use the *netCDF* [22] file format. Use these to save data for 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 a continuous `FunctionSpace` to the file `x.nc` use

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

To recover the object `x`, and you know that `mydomain` was an `esys.finley` mesh, use

```
from esys.finley import LoadMesh
mydomain=LoadMesh("dom.nc")
x=load("x.nc", mydomain)
```

Obviously, it is possible to execute the same steps that were originally used to generate `mydomain` to recreate it. However, in most cases using `dump` and `load` is faster, particularly if optimization has been applied. If `esys.escript` is running on more than one *MPI* process `dump` will create an individual file for each process containing the local data. In order to avoid conflicts the file names are extended by the *MPI* processor rank, that is instead of one file `dom.nc` you would get `dom.nc.0000`, `dom.nc.0001`, etc. You still call `LoadMesh("dom.nc")` to load the domain but you have to make sure that the appropriate file is accessible from the corresponding rank, and loading will only succeed if you run with as many processes as were used when calling `dump`.

The function space of the `Data` is stored in `x.nc`. 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 reordered so be aware and confirm that you get what you wanted.

A newer, more flexible way of saving and restoring `esys.escript` simulation data is through an instance of the `DataManager` class. It has the advantage of allowing to save and load not only a `Domain` and `Data` objects but also other values[1] you compute in your simulation script. Further, `DataManager` objects can simultaneously create files for visualization so no extra calls to `saveVTK` etc. are needed.

The following example shows how the `DataManager` class can be used. For an explanation of all member functions and options see the class reference section 3.2.8.

[1] The *python pickle* module is used for other types.

```
from esys.escript import DataManager, Scalar, Function
from esys.finley import Rectangle

dm = DataManager(formats=[DataManager.RESTART, DataManager.VTK])
if dm.hasData():
  mydomain=dm.getDomain()
  val=dm.getValue("val")
  t=dm.getValue("t")
  t_max=dm.getValue("t_max")
else:
  mydomain=Rectangle()
  val=Function(mydomain).getX()
  t=0.
  t_max=2.5

while t<t_max:
  t+=.01
  val=val+t/2
  dm.addData(val=val, t=t, t_max=t_max)
  dm.export()
```

In the constructor we specify that we want `RESTART` (i.e. dump) files and `VTK` files to be saved. By default, the constructor will look for previously saved `RESTART` files under the current directory and load them. We can then enquire if such files were found by calling the `hasData` method. If it returns *True* we retrieve the domain and values into local variables. Otherwise the same variables are initialized with appropriate values to start a new simulation. Note, that `t` and `t_max` are regular floating point values and not `Data` objects. Yet they are treated the same way by the `DataManager`.

After this initialization step the script enters the main simulation loop where calculations are performed. When these are finalized for a time step we call the `addData` method to let the manager know which variables to store on disk. This does not actually save the data yet and it is allowed to call `addData` more than once to add information incrementally, e.g. from separate functions that have access to the `DataManager` instance. Once all variables have been added the `export` method has to be called to flush all data to disk and clear the manager. In this example, this call dumps `mydomain` and `val` to files in a restart directory and also stores `t` and `t_max` on disk. Additionally, it generates a *VTK* file for visualization of the data. If the script would stop running before its completion for some reason (e.g. because its runtime limit was exceeded in a multiuser environment), you could simply run it again and it would resume at the point it stopped before.

3.2 `esys.escript` Classes

3.2.1 The `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`.

dump(filename)

writes the `Domain` to the file `filename` using the *netCDF* file format.

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 new locations 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 a `Data` object.

getSize()
returns the local sample size, i.e. the element diameter, as a `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)
returns *True* if `tag_name` is a valid tag name.

__eq__(arg)
(*python* == operator) returns *True* if the `Domain` `arg` describes the same domain, *False* otherwise.

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

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

onMasterProcessor)()
returns *True* if the processor is the master processor within the *MPI* processor group used by the `Domain`. This is the processor with rank 0. If *MPI* support is not enabled the return value is always *True*.

getMPISize()
returns the number of *MPI* processors used for this `Domain`. If *MPI* support is not enabled 1 is returned.

getMPIRank()
returns the rank of the processor executing the statement within the *MPI* processor group used by the `Domain`. If *MPI* support is not enabled 0 is returned.

MPIBarrier()
executes barrier synchronization within the *MPI* processor group used by the `Domain`. If *MPI* support is not enabled, this command does nothing.

3.2.2 The `FunctionSpace` class

class FunctionSpace()
`FunctionSpace` objects, which are instantiated by generator functions, are used to define properties of `Data` objects such as continuity. 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 hyper-manifold (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` object 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 samples where `mask` is positive for a least one data point. `mask` must be defined on this `FunctionSpace`. Use the `setTagMap` to assign a tag name to `new_tag`.

__eq__(arg)
(*python* == operator) returns *True* if the `FunctionSpace` `arg` describes the same function space, *False* otherwise.

__ne__(arg)
(*python* `!=` operator) returns *True* if the `FunctionSpace` `arg` does not describe the same function space, *False* otherwise.

__str__()
(*python* `str()` function) returns a string representation of the `FunctionSpace`.

The following functions 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 boundary `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 the 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 the geometric region defined by `domain` and are solutions of partial differential equations with a reduced smoothness for the solution approximation.

3.2.3 The `Data` Class

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

Expression	Description
`+arg`	identical to `arg`
`-arg`	negation of `arg`
`arg0+arg1`	adds `arg0` and `arg1`
`arg0*arg1`	multiplies `arg0` and `arg1`
`arg0-arg1`	subtracts `arg1` from `arg0`
`arg0/arg1`	divides `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 `numpy` 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+=arg1`	adds `arg1` to `arg0`
`arg0*=arg1`	multiplies `arg0` by `arg1`
`arg0-=arg1`	subtracts `arg1` from`arg0`
`arg0/=arg1`	divides `arg0` by `arg1`
`arg0**=arg1`	raises `arg0` to the power of `arg1`

`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 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	N/A
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)

Let `s` be the shape of `arg`, then

$$0 \le l0 \le u0 \le s[0],$$
$$0 \le l1 \le u1 \le s[1],$$
$$0 \le l2 \le u2 \le s[2],$$
$$0 \le l3 \le u3 \le s[3].$$

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 omitted, 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]
```

3.2.4 Generation of Data objects

class Data(value=0, shape=(,), what=FunctionSpace(), expanded=*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 form.

class Data(value, what=FunctionSpace(), expanded=*False*)
creates a Data object in the FunctionSpace what. The value for each data sample point is set to value, which could be a numpy object, Data object or a dictionary of numpy 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(), expanded=*False*)
returns a Data object of rank 0 (a constant) in the FunctionSpace what. Values are initialized with value, a double precision quantity. If expanded is *True* the Data object is represented in expanded form.

Vector(value=0., what=FunctionSpace(), expanded=*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 initialized with value, a double precision quantity. If expanded is *True* the Data object is represented in expanded form.

Tensor(value=0., what=FunctionSpace(), expanded=*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 initialized with value, a double precision quantity. If expanded is *True* the Data object is represented in expanded form.

Tensor3(value=0., what=FunctionSpace(), expanded=*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 initialized with value, a double precision quantity. If expanded is *True* the Data object is represented in expanded form.

Tensor4(value=0., what=FunctionSpace(), expanded=*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 initialized with value, a double precision quantity. If expanded is *True* the Data object is represented in expanded form.

load(filename, domain)

recovers a Data object on Domain domain from the file filename, which was created by dump.

3.2.5 Data methods

These are the most frequently used methods of the Data class. A complete list of methods can be found on http://esys.esscc.uq.edu.au/docs.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* if the Data object is the empty Data object, *False* otherwise. 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 numpy.ndarray or must be convertible into a numpy.ndarray object. value (or the corresponding numpy.ndarray object) must be of rank 0 or must have the same rank as the object. If a value has already been 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 value is assigned the 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 the responsibility of the user to save the Domain in order to be able to recover the Data object.

__str__()
returns a string representation of the object.

3.2.6 Functions of Data objects

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

saveVTK(filename, **kwdata)
writes Data defined by keywords to the file filename using the *VTK* file format. The keyword is used as an identifier. The statement

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

writes the scalar T as temperature and the vector v as velocity into the file out.vtu. Restrictions on the allowed combinations of FunctionSpace apply. This method is deprecated and will be removed in a future version of escript. Use the weipa module instead!

saveDX(filename, **kwdata)
writes Data defined by keywords to the file filename using the *OpenDX*[23] file format. The keyword is used as an identifier. The statement

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

writes 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) `numpy` 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) `numpy` 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 $(d,)$ `numpy` 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 point the minimum value over all components.

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

length(a)
returns the Euclidean norm at each data sample point. For a rank-4 `Data` object `a` this is

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

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 this is

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

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

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

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. For instance, in the case of a rank-2 Data object this is

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

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

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

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. For instance, if a is a rank-4 Data object, axis0=1 and axis1=2, the result is

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

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 so that

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

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

eigenvalues(a)
returns the eigenvalues of a so that

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

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

eigenvalues_and_eigenvectors(a)
returns the eigenvalues and eigenvectors of a.

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

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

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

if a has shape (d,d). The eigenvalues are ordered in increasing size. The argument a has to be the symmetric, i.e. 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.

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

at all data sample points.

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

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

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 a rank-2 Data object:

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

and for a rank-4 Data object:

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

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

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

and if a1 is a rank-2 Data object this is

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

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 a rank-1 Data object this is

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

and if a1 is a rank-2 Data object this is

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

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 a rank-2 `Data` object this is

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

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

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

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

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

tensor_mult(a0,a1)
returns the tensor product of `a0` and `a1`. If `a1` is a rank-2 `Data` object this is

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

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

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

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 a rank-2 `Data` object this is

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

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

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

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 a rank-2 `Data` object this is

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

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

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

grad(a[, where=None])
returns the gradient of `a`. If `where` is present the gradient will be calculated in the `FunctionSpace` `where`, otherwise a default `FunctionSpace` is used. In case that `a` is a rank-2 `Data` object one has

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

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 in continuous `FunctionSpace` it is

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

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`:

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

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

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

L2(a)
returns the L^2-norm of `a` in its `FunctionSpace`. 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 the sine function to `a`.

cos(a)
applies the cosine function to `a`.

tan(a)
applies the tangent function to `a`.

asin(a)
applies the arc (inverse) sine function to `a`.

acos(a)
applies the arc (inverse) cosine function to `a`.

atan(a)
applies the arc (inverse) tangent function to `a`.

sinh(a)
applies the hyperbolic sine function to `a`.

cosh(a)
applies the hyperbolic cosine function to `a`.

tanh(a)
applies the hyperbolic tangent function to `a`.

asinh(a)
applies the arc (inverse) hyperbolic sine function to `a`.

acosh(a)
applies the arc (inverse) hyperbolic cosine function to `a`.

atanh(a)
applies the arc (inverse) hyperbolic tangent function to `a`.

exp(a)
applies the exponential function to `a`.

sqrt(a)
applies the square root function to `a`.

log(a)
takes the natural logarithm of `a`.

log10(a)
takes the base-10 logarithm of `a`.

sign(a)
applies the sign function to `a`. The result 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=None, [, rtol=1.e-8]])
returns a function which is 1 where `a` equals zero with tolerance `tol` and 0 otherwise. If `tol` is not present, the absolute maximum value of `a` times `rtol` is used.

whereNonZero(a, [, tol=None, [, rtol=1.e-8]])
returns a function which is 1 where `a` is non-zero with tolerance `tol` and 0 otherwise. If `tol` is not present, the absolute maximum value of `a` times `rtol` is used.

3.2.7 Interpolating Data

In some cases, it may be useful to produce Data objects which fit some user defined function. Manually modifying each value in the Data object is not a good idea since it depends on knowing the location and order of each data point in the domain. Instead, `esys.escript` can use an interpolation table to produce a `Data` object.

The following example is available as `int_save.py` in the example directory. We will produce a `Data` object which approximates a sine curve.

```
from esys.escript import saveDataCSV, sup, interpolateTable
import numpy
from esys.finley import Rectangle

n=4
r=Rectangle(n,n)
x=r.getX()
toobig=100
```

First we produce an interpolation table:

```
sine_table=[0, 0.70710678118654746, 1, 0.70710678118654746, 0,
            -0.70710678118654746, -1, -0.70710678118654746, 0]
```

We wish to identify 0 and 1 with the ends of the curve, that is with the first and eighth value in the table.

```
numslices=len(sine_table)-1
minval=0.
maxval=1.
step=sup(maxval-minval)/numslices
```

So the values v from the input lie in the interval `minval` $\leq v <$ `maxval`. `step` represents the gap (in the input range) between entries in the table. By default, values of v outside the table argument range (minval, maxval) will be pushed back into the range, i.e. if $v <$ `minval` the value `minval` will be used to evaluate the table. Similarly, for values $v >$ `maxval` the value `maxval` is used.

Now we produce our new `Data` object:

```
result=interpolateTable(sine_table, x[0], minval, step, toobig)
```

Any values which interpolate to larger than `toobig` will raise an exception. You can switch on boundary checking by adding `check_boundaries=True` to the argument list.

Now consider a 2D example. We will interpolate from a plane where $\forall x, y \in [0, 9] : (x, y) = x + y \cdot 10$.

```
from esys.escript import whereZero
table2=[]
for y in range(0,10):
      r=[]
      for x in range(0,10):
         r.append(x+y*10)
      table2.append(r)
xstep=(maxval-minval)/(10-1)
ystep=(maxval-minval)/(10-1)

xmin=minval
ymin=minval

result2=interpolateTable(table2, x2, (xmin, ymin), (xstep, ystep), toobig)
```

We can check the values using `whereZero`. For example, for $x = 0$:

```
print result2*whereZero(x[0])
```

Now a 3D. Note that the parameter tuples should be (x, y, z) but that in the interpolation table, x is the innermost dimension.

```
b=Brick(n,n,n)
x3=b.getX()
toobig=1000000
```

```
table3=[]
for z in range(0,10):
   face=[]
   for y in range(0,10):
      r=[]
      for x in range(0,10):
         r.append(x+y*10+z*100)
      face.append(r)
   table3.append(face);

zstep=(maxval-minval)/(10-1)

zmin=minval

result3=interpolateTable(table3, x3, (xmin, ymin, zmin), (xstep, ystep, zstep), toobig)
```

3.2.8 The `DataManager` Class

class DataManager(formats=[RESTART], work_dir=".", **restart_prefix="restart"**, **do_restart=*True*)**

initializes a new `DataManager` object which can be used to save, restore and export simulation data in a number of formats. All files and directories saved or restored by this object are located under the directory specified by `work_dir`. If `RESTART` is specified in `formats`, the `DataManager` will look for directories whose name starts with `restart_prefix`. In case `do_restart` is *True*, the last of these directories is used to restore simulation data while all others are deleted. If `do_restart` is *False*, then all of those directories are deleted. The `restart_prefix` and `do_restart` parameters are ignored if `RESTART` is not specified in `formats`.

Valid values for the `formats` parameter are:

RESTART

enables writing of checkpoint files to be able to continue simulations as explained in the class description.

SILO

exports simulation data in the *SILO* file format. `esys.escript` must have been compiled with *SILO* support for this to work.

VISIT

enables the *VisIt* simulation interface which allows connecting to and interacting with the running simulation from a compatible *VisIt* client. `esys.escript` must have been compiled with *VisIt* (version 2) support and the version of the client has to match the version used at compile time. In order to connect to the simulation the client needs to have access and load the file `escriptsim.sim2` located under the work directory.

VTK

exports simulation data in the *VTK* file format.

The `DataManager` class has the following methods:

addData(data)**

adds `Data` objects and other data to the manager. Calling this method does not save or export the data yet so it is allowed to incrementally add data at various points in the simulation script if required. Note, that only a single domain is supported so all `Data` objects have to be defined on the same one or an exception is raised.

setDomain(domain)

explicitly sets the domain for this manager. It is generally not required to call this method directly. Instead, the `addData` method will set the domain used by the `Data` objects. An exception is raised if the domain was set to a different domain before (explicitly or implicitly).

hasData()
returns *True* if the manager has loaded simulation data for a restart.

getDomain()
returns the domain as recovered from a restart.

getValue(value_name)
returns a `Data` object or other value with the name `value_name` that has been recovered after a restart.

getCycle()
returns the export cycle, i.e. the number of times `export()` has been called.

setCheckpointFrequency(freq)
sets the frequency with which checkpoint files are created. This is only useful if the `DataManager` object was created with at least one other format next to `RESTART`. The frequency is 1 by default which means that checkpoint files are created every time `export()` is called. Unlike visualization output, a simulation checkpoint is usually not required at every time step. Thus, the frequency can be decreased by calling this method with `freq` > 1 which would then create restart files every `freq` times `export()` is called.

setTime(time)
sets the simulation time stamp. This floating point number is stored in the metadata of exported data but not used by `RESTART`.

setMeshLabels(x, y, z="")
sets labels for the mesh axes. These are currently only used by the *SILO* exporter.

setMeshUnits(x, y, z="")
sets units for the mesh axes. These are currently only used by the *SILO* exporter.

setMetadataSchemaString(schema, metadata="")
sets metadata namespaces and the corresponding metadata. These are currently only used by the *VTK* exporter. `schema` is a dictionary that maps prefixes to namespace names, e.g. {`"gml": "http://www.opengis.net/gml"`} and `metadata` is a string with the actual content which will be enclosed in `<MetaData>` tags.

export()
executes the actual data export. Depending on the `formats` parameter used in the constructor all data added by `addData()` is written to disk (`RESTART,SILO,VTK`) or made available through the *VisIt* simulation interface (`VISIT`). At least the domain must be set for something to be exported.

3.2.9 Saving Data as CSV

For simple post-processing, `Data` objects can be saved in comma separated value (*CSV*) format. If `mydata1` and `mydata2` are scalar data, the command

```
saveDataCSV('output.csv', U=mydata1, V=mydata2)
```

will record the values in `output.csv` in the following format:

```
U, V
1.0000000e+0, 2.0000000e-1
5.0000000e-0, 1.0000000e+1
...
```

The names of the keyword parameters form the names of columns in the output. If the data objects are over different function spaces, then `saveDataCSV` will attempt to interpolate to a common function space. If this is not possible, then an exception is raised.

Output can be restricted using a scalar mask as follows:

```
saveDataCSV('outfile.csv', U=mydata1, V=mydata2, mask=myscalar)
```

This command will only output those rows which correspond to to positive values of `myscalar`. Some aspects of the output can be tuned using additional parameters:

```
saveDataCSV('data.csv', append=True, sep=' ', csep='/', mask=mymask, e=mat1)
```

- `append` – specifies that the output should be written to the end of an existing file
- `sep` – defines the separator between fields
- `csep` – defines the separator between components in the header line. For example between the components of a matrix.

The above command would produce output like this:

```
e/0/0 e/1/0 e/0/1 e/1/1
1.0000000000e+00 2.0000000000e+00 3.0000000000e+00 4.0000000000e+00
...
```

Note that while the order in which rows are output can vary, all the elements in a given row always correspond to the same input.

3.2.10 The `Operator` Class

The `Operator` class provides an abstract access to operators built 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, *False* otherwise.

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 with name `fileName`, see http://maths.nist.gov/MatrixMarket

3.3 Physical Units

`esys.escript` provides support for physical units in the SI system including unit conversion. So the user can define variables in the form

```
from esys.escript.unitsSI import *
l=20*m
w=30*kg
w2=40*lb
T=100*Celsius
```

In the two latter cases a conversion from pounds and degrees Celsius is performed into the appropriate SI units *kg* and *Kelvin*. In addition, composed units can be used, for instance

```
from esys.escript.unitsSI import *
rho=40*lb/cm**3
```

defines the density in the units of pounds per cubic centimeter. The value 40 will be converted into SI units, in this case kg per cubic meter. Moreover unit prefixes are supported:

```
from esys.escript.unitsSI import *
p=40*Mega*Pa
```

The pressure `p` is set to 40 Mega Pascal. Units can also be converted back from the SI system into a desired unit, e.g.

```
from esys.escript.unitsSI import *
print p/atm
```

can be used print the pressure in units of atmosphere.

The following is an incomplete list of supported physical units:

km
: unit of kilometer

m
: unit of meter

cm
: unit of centimeter

mm
: unit of millimeter

sec
: unit of second

minute
: unit of minute

h
: unit of hour

day
: unit of day

yr
: unit of year

gram
: unit of gram

kg
: unit of kilogram

lb
unit of pound

ton
metric ton

A
unit of Ampere

Hz
unit of Hertz

N
unit of Newton

Pa
unit of Pascal

atm
unit of atmosphere

J
unit of Joule

W
unit of Watt

C
unit of Coulomb

V
unit of Volt

F
unit of Farad

Ohm
unit of Ohm

K
unit of degrees Kelvin

Celsius
unit of degrees Celsius

Fahrenheit
unit of degrees Fahrenheit

Supported unit prefixes:

Yotta
prefix yotta = 10^{24}

Zetta
prefix zetta = 10^{21}

Exa
prefix exa = 10^{18}

Peta
prefix peta = 10^{15}

Tera
prefix tera = 10^{12}

Giga
prefix giga = 10^{9}

Mega
prefix mega = 10^{6}

Kilo
prefix kilo = 10^{3}

Hecto
prefix hecto = 10^{2}

Deca
prefix deca = 10^{1}

Deci
prefix deci = 10^{-1}

Centi
prefix centi = 10^{-2}

Milli
prefix milli = 10^{-3}

Micro
prefix micro = 10^{-6}

Nano
prefix nano = 10^{-9}

Pico
prefix pico = 10^{-12}

Femto
prefix femto = 10^{-15}

Atto
prefix atto = 10^{-18}

Zepto
prefix zepto = 10^{-21}

Yocto
prefix yocto = 10^{-24}

3.4 Utilities

The `FileWriter` class provides a mechanism to write data to a file. In essence, this class wraps the standard *python* `file` class to write data that are global in *MPI* to a file. In fact, data are written on the processor with *MPI* rank 0 only. It is recommended to use `FileWriter` rather than `open` in order to write code that will run with and without *MPI*. It is safe to use `open` under *MPI* to *read* data which are global under *MPI*.

class FileWriter(fn[,append=*False*, [createLocalFiles=*False*]])

Opens a file with name `fn` for writing. If `append` is set to *True* data are appended at the end of the file. If running under *MPI*, only the first processor (rank==0) will open the file and write to it. If `createLocalFiles` is set each individual processor will create a file where for any processor with rank¿0 the file name is extended by its rank. This option is normally used for debugging purposes only.

The following methods are available:

close()
closes the file.

flush()
flushes the internal buffer to disk.

write(txt)
writes string `txt` to the file. Note that a newline is not added.

writelines(txts)
writes the list `txts` of strings to the file. Note that newlines are not added. This method is equivalent to calling `write()` for each string.

closed
this member is *True* if the file is closed.

mode
holds the access mode.

name
holds the file name.

newlines
holds the line separator.

setEscriptParamInt(name,value)
assigns the integer value `value` to the parameter `name`. If `name` ="TOO_MANY_LINES" conversion of any `Data` object to a string switches to a condensed format if more than `value` lines would be created.

getEscriptParamInt(name)
returns the current value of integer parameter `name`.

listEscriptParams(a)
returns a list of valid parameters and their description.

getMPISizeWorld()
returns the number of *MPI* processors in use in the **MPI_COMM_WORLD** processor group. If *MPI* is not used 1 is returned.

getMPIRankWorld()
returns the rank of the current process within the **MPI_COMM_WORLD** processor group. If *MPI* is not used 0 is returned.

MPIBarrierWorld()
performs a barrier synchronization across all processors within the **MPI_COMM_WORLD** processor group.

getMPIWorldMax(a)
returns the maximum value of the integer `a` across all processors within **MPI_COMM_WORLD**.

CHAPTER
FOUR

The `esys.escript.linearPDEs` Module

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 and n denotes the outer normal field on Γ.

For a single PDE with a solution that has 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, i.e. summation over indexes appearing twice in a term of a sum, is used in this chapter. 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 each a rank-1 `Data` object and D and Y are scalars. 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 prescribe 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 a 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 a rank-1 `Data` object. Notice that not necessarily all components must have a constraint at all locations.

`LinearPDE` also supports solution discontinuities over a contact region $\Gamma^{contact}$ in the domain Ω. To specify the conditions across the discontinuity we are using the generalised flux J[1] which in the case of a system of PDEs and several components of the solution, is 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 as

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

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 the 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 coefficient $d^{contact}$ and $y^{contact}$ are each a 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 to the scalar case Equation (4.11) now the coefficients D, d and $d^{contact}$ have to be inspected.

The following example illustrates a typical usage of the `LinearPDE` class:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE
from esys.finley import Rectangle
mydomain = Rectangle(l0=1., l1=1., n0=40, n1=20)
mypde=LinearPDE(mydomain)
mypde.setSymmetryOn()
mypde.setValue(A=kappa*kronecker(mydomain), D=1, Y=1)
u=mypde.getSolution()
```

We refer to Chapter 1 for more details.

An instance of the `SolverOptions` class is attached to the `LinearPDE` class object. It holds options for the solver that may be set before solving the PDE. In the following example the `getSolverOptions` method is used to access the `SolverOptions` object attached to `mypde`:

```
from esys.escript import *
from esys.escript.linearPDEs import LinearPDE, SolverOptions
from esys.finley import Rectangle
mydomain = Rectangle(l0=1., l1=1., n0=40, n1=20)
mypde=LinearPDE(mydomain)
mypde.setValue(A=kappa*kronecker(mydomain), D=1, Y=1)
```

[1] In some applications the definition of flux used here can be different from the commonly used definition. For instance, if T is a temperature field the heat flux q is defined as $q_{,i} = -\kappa T_{,i}$ (κ is the diffusivity) which differs from the definition used here by the sign. This needs to be kept in mind when defining natural boundary conditions.

```
mypde.getSolverOptions().setVerbosityOn()
mypde.getSolverOptions().setSolverMethod(SolverOptions.PCG)
mypde.getSolverOptions().setPreconditioner(SolverOptions.AMG)
mypde.getSolverOptions().setTolerance(1e-8)
mypde.getSolverOptions().setIterMax(1000)
u=mypde.getSolution()
```

In this example, the preconditioned conjugate gradient method `SolverOptions.PCG` is used with preconditioner `SolverOptions.AMG` . The relative tolerance is set to 10^{-8} and the maximum number of iteration steps to 1000. After a completed call to `getSolution()`, the attached `SolverOptions` object gives access to diagnostic information:

```
u=mypde.getSolution()
print("Number of iteration steps =", mypde.getDiagnostics("num_iter"))
print("Total solution time =", mypde.getDiagnostics("time"))
print("Set-up time =", mypde.getDiagnostics("set_up_time"))
print("Net time =", mypde.getDiagnostics("net_time"))
print("Residual norm of returned solution =", mypde.getDiagnostics('residual_norm'))
```

Typically, a negative value for a diagnostic variable indicates that it is undefined.

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, e.g. `esys.finley`. The general interface is provided through the `LinearPDE` class. 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://esys.esscc.uq.edu.au/docs.html.

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

4.1.2.1 `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[2]. If the new coefficient value is not a `Data` object, it is converted into a `Data` object in the appropriate `FunctionSpace`.

getCoefficient(name)
returns the value assigned to coefficient `name`. If `name` is not a valid name an exception is raised.

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

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

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

setDebugOn()
switches on debug mode so more diagnostic messages will be printed.

setDebugOff()
switches off debug mode.

getSolverOptions()
returns the solver options for solving the PDE. In fact, the method returns a `SolverOptions` class object which can be used to modify the tolerance, the solver or the preconditioner, see Section 4.3 for details.

setSolverOptions([options=None])
sets the solver options for solving the PDE. If argument `options` is present it must be a `SolverOptions` class object, see Section 4.3 for details. Otherwise the solver options are reset to the default.

isUsingLumping()
returns *True* if matrix lumping is set as the solver for the system of linear equations, *False* otherwise.

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, *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 is printed.

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

isSymmetric()
returns *True* if the PDE has been indicated to be symmetric, *False* otherwise.

setSymmetryOn()
indicates that the PDE is symmetric.

setSymmetryOff()
indicates that the PDE is not symmetric.

setReducedOrderOn()
enables 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()
disables 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()
returns (an approximation of) the solution of the PDE. This call will invoke the discretization of the PDE and the solution of the resulting system of linear equations. Keep in mind that this call is typically computationally expensive and – depending on the PDE and the discretization – can take a long time to complete.

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, and f each 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`, and `q`. By default all values are set to zero.

4.1.5 The `Lame` Class

The `Lame` class defines a Lame equation problem

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

with natural boundary conditions

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

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 zero.

4.2 Projection

Using the `LinearPDE` class provides an option to change the `FunctionSpace` attribute in addition to the standard interpolation mechanism as discussed in Chapter 3. If you consider the stripped-down version

$$u = Y \tag{4.26}$$

of the general scalar PDE 4.1 (boundary conditions are irrelevant), you can see the solution u of this PDE as a projection of the input function Y which has the general `FunctionSpace` attribute to a function with the solution `FunctionSpace` or reduced solution `FunctionSpace` attribute. In fact, the solution maps values defined at element centers representing a possibly discontinuous function onto a continuous function represented by its values at the nodes of the FEM mesh. This mapping is called a projection. Projection can be a useful tool but needs to be applied with some care due to the possibility of projecting a potentially discontinuous function onto a continuous function, although this may also be a desirable effect, for instance to smooth a function. The projection of the gradient of a function typically calculated on the element center to the nodes of a FEM mesh can be evaluated on the domain boundary and so projection provides a tool to extrapolate the gradient from the internal to the boundary. This is only a reasonable procedure in the absence of singularities at the boundary.

As projection is often used in simulations `esys.escript` provides an easy to use class `Projector` which is part of the `esys.escript.pdetools` module. The following script demonstrates the usage of the class to project the piecewise constant function ($= 1$ for $x_0 \geq 0.5$ and $= -1$ for $x_0 < 0.5$) to a function with the reduced solution `FunctionSpace` attribute (default target):

```
from esys.escript.pdetools import Projector
proj=Projector(domain)
x0=domain.getX()[0]
jmp=1.-2.*wherePositive(x0-0.5)
u=proj.getValue(jmp)
# alternative call:
u=proj(jmp)
```

By default the class uses lumping to solve the PDE 4.26. This technique is faster than using the standard solver techniques of PDEs. In essence it leads to using the average of neighbour element values to calculate the value at each FEM node.

The following script illustrates how to evaluate the normal stress on the boundary from a given displacement field `u`:

```
from esys.escript.pdetools import Projector
u=...
proj=Projector(u.getDomain())
e=symmetric(grad(u))
stress = G*e+ (K-2./3.*G)*trace(e)*kronecker(u.getDomain())
normal_stress = inner(u.getDomain().getNormal(), proj(stress))
```

class Projector(domain[, reduce=*True* [, fast=*True*]])
This class defines a projector on the domain `domain`. If `reduce` is set to *True* the projection will be returned as a reduced solution `FunctionSpace Data` object. Otherwise the solution `FunctionSpace` representation is returned. If `reduce` is set to *True* lumping is used when the Equation (4.26) is solved, otherwise the standard PDE solver is used. Notice, that lumping requires significantly less computation time and memory. The class is callable.

getSolverOptions()
returns the solver options for solving the PDE. In fact, the method returns a `SolverOptions` class object which can be used to modify the tolerance, the solver or the preconditioner, see Section 4.3 for details.

getValue(input_data)
projects the `input_data`. This method is equivalent to call an instance of the class with argument `input_data`

4.3 Solver Options

class SolverOptions()
This class defines the solver options for a linear or non-linear solver. The option also supports the handling of diagnostic information.

getSummary()
returns a string reporting the current settings.

getName(key)
returns the name as a string of a given key.

setSolverMethod([method=SolverOptions.DEFAULT])
sets the solver method to be used. Use `method` =`SolverOptions.DIRECT` to indicate that a direct rather than an iterative solver should be used and use `method` =`SolverOptions.ITERATIVE` to indicate that an iterative rather than a direct solver should be used. The value of `method` must be one of the constants:
`SolverOptions.DEFAULT`
`SolverOptions.DIRECT`
`SolverOptions.CHOLEVSKY`
`SolverOptions.PCG`
`SolverOptions.CR`
`SolverOptions.CGS`
`SolverOptions.BICGSTAB`
`SolverOptions.SSOR`
`SolverOptions.GMRES`
`SolverOptions.PRES20`
`SolverOptions.ROWSUM_LUMPING`
`SolverOptions.HRZ_LUMPING`
`SolverOptions.ITERATIVE`
`SolverOptions.NONLINEAR_GMRES`
`SolverOptions.TFQMR`

`SolverOptions.MINRES`
`SolverOptions.GAUSS_SEIDEL`.
Not all packages support all solvers. It can be assumed that a package makes a reasonable choice if it encounters an unknown solver. See Table 7.2 for the solvers supported by `esys.finley`.

getSolverMethod()
returns the key of the solver method to be used.

setPreconditioner([preconditioner=SolverOptions.JACOBI])
sets the preconditioner to be used. The value of `preconditioner` must be one of the constants:
`SolverOptions.ILU0`
`SolverOptions.JACOBI`
`SolverOptions.AMG`
`SolverOptions.REC_ILU`
`SolverOptions.GAUSS_SEIDEL`
`SolverOptions.RILU`
`SolverOptions.NO_PRECONDITIONER`.
Not all packages support all preconditioners. It can be assumed that a package makes a reasonable choice if it encounters an unknown preconditioner. See Table 7.3 for the preconditioners supported by `esys.finley`.

getPreconditioner()
returns the key of the preconditioner to be used.

setPackage([package=SolverOptions.DEFAULT])
sets the solver package to be used as a solver. The value of `method` must be one of the constants:
`SolverOptions.DEFAULT`
`SolverOptions.PASO`
`SolverOptions.SUPER_LU`
`SolverOptions.PASTIX`
`SolverOptions.MKL`
`SolverOptions.UMFPACK`.
Not all packages are supported on all implementations. An exception may be thrown on some platforms if a particular package is requested. Currently `esys.finley` supports `SolverOptions.PASO` (as default) and, if available, `SolverOptions.MKL`[3] and `SolverOptions.UMFPACK`.

getPackage()
returns the solver package key.

resetDiagnostics([all=False])
resets the diagnostics. If `all` is *True* all diagnostics, including accumulative counters, are reset.

getDiagnostics([name])
returns the diagnostic information `name`. The following keywords are supported:
`"num_iter"`: number of iteration steps
`"cum_num_iter"`: cumulative number of iteration steps
`"num_level"`: number of levels in the multi level solver
`"num_inner_iter"`: number of inner iteration steps
`"cum_num_inner_iter"`: cumulative number of inner iteration steps
`"time"`: execution time
`"cum_time"`: cumulative execution time
`"set_up_time"`: time to set up the solver, typically this includes factorization and reordering
`"cum_set_up_time"`: cumulative time to set up the solver

[3] If the stiffness matrix is non-regular `MKL` may return without returning a proper error code. If you observe suspicious solutions when using MKL, this may be causes by a non-invertible operator.

"net_time": net execution time, excluding setup time for the solver and execution time for preconditioner
"cum_net_time": cumulative net execution time
"residual_norm": norm of the final residual
"converged": status of convergence
"preconditioner_size": size of preconditioner in MBytes
"preconditioner_size": size of preconditioner in MBytes
"preconditioner_size": size of preconditioner in MBytes .

hasConverged()
returns *True* if the last solver call has been finalized successfully. If an exception has been thrown by the solver the status of this flag is undefined.

setReordering([ordering=SolverOptions.DEFAULT_REORDERING])
sets the key of the reordering method to be applied if supported by the solver. Some direct solvers support reordering to optimize compute time and storage use during elimination. The value of `ordering` must be one of the constants:
`SolverOptions.NO_REORDERING`
`SolverOptions.MINIMUM_FILL_IN`
`SolverOptions.NESTED_DISSECTION`
`SolverOptions.DEFAULT_REORDERING`.

getReordering()
returns the key of the reordering method to be applied if supported by the solver.

setRestart([restart=None])
sets the number of iterations steps after which `SolverOptions.GMRES` is to perform a restart. If `restart` is equal to `None` no restart is performed.

getRestart()
returns the number of iterations steps after which `SolverOptions.GMRES` performs a restart.

setTruncation([truncation=20])
sets the number of residuals in `SolverOptions.GMRES` to be stored for orthogonalization. The more residuals are stored the faster `SolverOptions.GMRES` converges but the higher the storage needs are and the more expensive a single iteration step becomes.

getTruncation()
returns the number of residuals in `SolverOptions.GMRES` to be stored for orthogonalization.

setIterMax([iter_max=10000])
sets the maximum number of iteration steps.

getIterMax()
returns maximum number of iteration steps.

setLevelMax([level_max=10])
sets the maximum number of coarsening levels to be used in the `SolverOptions.AMG` solver or preconditioner.

getLevelMax()
returns the maximum number of coarsening levels to be used in an algebraic multi level solver or preconditioner.

setCoarseningThreshold([theta=0.25])
sets the threshold for coarsening in the `SolverOptions.AMG` solver or preconditioner.

getCoarseningThreshold()
returns the threshold for coarsening in the `SolverOptions.AMG` solver or preconditioner.

setDiagonalDominanceThreshold([value=0.5])
sets the threshold for diagonal dominant rows which are eliminated during `SolverOptions.AMG` coarsening.

getDiagonalDominanceThreshold()
returns the threshold for diagonal dominant rows which are eliminated during `SolverOptions.AMG` coarsening.

setMinCoarseMatrixSize([size=500])
sets the minimum size of the coarsest level matrix in `SolverOptions.AMG`.

getMinCoarseMatrixSize()
returns the minimum size of the coarsest level matrix in `SolverOptions.AMG`.

setSmoother([smoother=`SolverOptions.GAUSS_SEIDEL`])
sets the `SolverOptions.JACOBI` or `SolverOptions.GAUSS_SEIDEL` smoother to be used with `SolverOptions.AMG`.

getSmoother()
returns the key of the smoother used in `SolverOptions.AMG`.

setAMGInterpolation([method=`None`])
sets interpolation method for `SolverOptions.AMG` to `CLASSIC_INTERPOLATION_WITH_FF_COUPLING`, `CLASSIC_INTERPOLATION`, or `DIRECT_INTERPOLATION`.

getAMGInterpolation()
returns the key `CLASSIC_INTERPOLATION_WITH_FF_COUPLING`, `CLASSIC_INTERPOLATION`, or `DIRECT_INTERPOLATION` of the interpolation method for `SolverOptions.AMG`.

setNumSweeps([sweeps=2])
sets the number of sweeps in a `SolverOptions.JACOBI` or `SolverOptions.GAUSS_SEIDEL` preconditioner.

getNumSweeps()
returns the number of sweeps in a `SolverOptions.JACOBI` or `SolverOptions.GAUSS_SEIDEL` preconditioner.

setNumPreSweeps([sweeps=2])
sets the number of sweeps in the pre-smoothing step of `SolverOptions.AMG`.

getNumPreSweeps()
returns the number of sweeps in the pre-smoothing step of `SolverOptions.AMG`.

setNumPostSweeps([sweeps=2])
sets the number of sweeps in the post-smoothing step of `SolverOptions.AMG`.

getNumPostSweeps()

returns he number of sweeps in the post-smoothing step of `SolverOptions.AMG`.

setTolerance([rtol=1.e-8])
sets the relative tolerance for the solver. The actual 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.

getTolerance()
returns the relative tolerance for the solver.

setAbsoluteTolerance([atol=0.])
sets the absolute tolerance for the solver. The actual 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.

getAbsoluteTolerance()
returns the absolute tolerance for the solver.

setInnerTolerance([rtol=0.9])
sets the relative tolerance for an inner iteration scheme, for instance on the coarsest level in a multi-level scheme.

getInnerTolerance()
returns the relative tolerance for an inner iteration scheme.

setRelaxationFactor([factor=0.3])
sets the relaxation factor used to add dropped elements in `SolverOptions.RILU` to the main diagonal.

getRelaxationFactor()
returns the relaxation factor used to add dropped elements in `SolverOptions.RILU` to the main diagonal.

isSymmetric()
returns *True* if the discrete system is indicated as symmetric.

setSymmetryOn()
sets the symmetry flag to indicate that the coefficient matrix is symmetric.

setSymmetryOff()
clears the symmetry flag for the coefficient matrix.

isVerbose()
returns *True* if the solver is expected to be verbose.

setVerbosityOn()
switches the verbosity of the solver on.

setVerbosityOff()
switches the verbosity of the solver off.

adaptInnerTolerance()
returns *True* if the tolerance of the inner solver is selected automatically. Otherwise the inner tolerance set by `setInnerTolerance` is used.

setInnerToleranceAdaptionOn()
switches the automatic selection of inner tolerance on.

setInnerToleranceAdaptionOff()
switches the automatic selection of inner tolerance off.

setInnerIterMax([iter_max=10])
sets the maximum number of iteration steps for the inner iteration.

getInnerIterMax()
returns the maximum number of inner iteration steps.

acceptConvergenceFailure()
returns *True* if a failure to meet the stopping criteria within the given number of iteration steps is not raising in exception. This is useful if a solver is used in a non-linear context where the non-linear solver can continue even if the returned solution does not necessarily meet the stopping criteria. One can use the `hasConverged` method to check if the last call to the solver was successful.

setAcceptanceConvergenceFailureOn()
switches the acceptance of a failure of convergence on.

setAcceptanceConvergenceFailureOff()
switches the acceptance of a failure of convergence off.

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.

MKL
the `MKL` library by Intel, Reference [18][4].

UMFPACK
the `UMFPACK` library, Reference [33]. Note that `UMFPACK` is not parallelized.

PASO
`PASO` is the default solver library of `esys.finley`, see Section 7.

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

DIRECT
the default direct linear solver.

CHOLEVSKY
direct solver based on Cholevsky factorization (or similar), see Reference [27]. The solver requires a symmetric PDE.

PCG
preconditioned conjugate gradient method, see Reference [36]. The solver requires a symmetric PDE.

TFQMR
transpose-free quasi-minimal residual method, see Reference [36].

[4]The `MKL` library will only be available when the Intel compilation environment was used to build `esys.escript`.

GMRES
the GMRES method, see Reference [36]. Truncation and restart are controlled by the `truncation` and `restart` parameters of `getSolution`.

MINRES
minimal residual method

ROWSUM_LUMPING
row sum lumping of the stiffness matrix, see Section **??** for details. Lumping does not use the linear system solver library.

HRZ_LUMPING
HRZ lumping of the stiffness matrix, see Section **??** for details. 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 [36].

CGS
conjugate gradient squared method, see Reference [36].

BICGSTAB
stabilized bi-conjugate gradients methods, see Reference [36].

SSOR
symmetric successive over-relaxation method, see Reference [36]. 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 [27].

JACOBI
the Jacobi preconditioner, see Reference [27].

AMG
the algebraic multi grid method, see Reference [28]. This method can be used as linear solver method but is more robust when used as a preconditioner.

GAUSS_SEIDEL
the symmetric Gauss-Seidel preconditioner, see Reference [27]. `getNumSweeps()` is the number of sweeps used.

REC_ILU
recursive incomplete LU factorization preconditioner, see Reference [32]. This method is similar to the one used for `SolverOptions.ILU0` but applies reordering during the factorization.

NO_REORDERING
no reordering is used during factorization.

DEFAULT_REORDERING
the default reordering method 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.

SUPER_LU
the SuperLU library [7] is used as a solver.

PASTIX
the Pastix library [13] is used as a solver.

NO_PRECONDITIONER
no preconditioner is applied.

DIRECT_INTERPOLATION
direct interpolation in `SolverOptions.AMG` , see [28]

CLASSIC_INTERPOLATION
classic interpolation in `SolverOptions.AMG` , see [28]

CLASSIC_INTERPOLATION_WITH_FF_COUPLING
classic interpolation with enforeced FF coupling in `SolverOptions.AMG` , see [28]

4.4 Some Remarks on Lumping

Explicit time integration schemes (two examples are discussed later in this section), require very small time steps in order to maintain numerical stability. Unfortunately, these small time increments often result in a prohibitive computational cost. In order to minimise these costs, a technique termed lumping can be utilised. Lumping is applied to the coefficient matrix, reducing it to a simple diagonal matrix. This can significantly improve the computational speed, because the solution updates are simplified to a simple component-by-component vector-vector product. However, some care is required when making radical approximations such as these. In this section, two commonly applied lumping techniques are discussed, namely row sum lumping and HRZ lumping .

4.4.1 Scalar wave equation

One example where lumping can be applied to a hyperpolic problem, is the scalar wave equation

$$u_{,tt} = c^2 u_{,ii} \ . \tag{4.27}$$

In this example, both of the lumping schemes are tested against the reference solution

$$u = sin(5\pi(x_0 - c * t)) \tag{4.28}$$

over the 2D unit square. Note that $u_{,i}n_i = 0$ on faces $x_1 = 0$ and $x_1 = 1$. Thus, on the faces $x_0 = 0$ and $x_0 = 1$ the solution is constrained.

To solve this problem the explicit Verlet scheme was used with a constant time step size dt given by

$$u^{(n)} = 2u^{(n-1)} - u^{(n-2)} + dt^2 a^{(n)} \tag{4.29}$$

for all $n = 2, 3, \ldots$ where the upper index (n) refers to values at time $t^{(n)} = t^{(n-1)} + h$ and $a^{(n)}$ is the solution of

$$a^{(n)} = c^2 u_{,ii}^{(n-1)} \ . \tag{4.30}$$

This equation can be interpreted as a PDE for the unknown value $a^{(n)}$, which must be solved at each time-step. In the notation of equation 4.1 we thus set $D = 1$ and $X = -c^2 u_{,i}^{(n-1)}$. Furthermore, in order to maintain stability, the time step size needs to fullfill the CourantFriedrichsLewy condition (CFL condition). For this example, the CFL condition takes the form

$$dt = f \cdot \frac{dx}{c}. \tag{4.31}$$

where dx is the mesh size and f is a safety factor. In this example, we use $f = \frac{1}{6}$.

Figure 4.1 depicts a temporal comparison between four alternative solution algorithms: the exact solution; using a full mass matrix; using HRZ lumping; and row sum lumping. The domain utilsed rectangular order 1

elements (element size is 0.01) with observations taken at the point $(\frac{1}{2}, \frac{1}{2})$. All four solutions appear to be identical for this example. This is not the case for order 2 elements, as illustrated in Figure 4.2. For the order 2 elements, the row sum lumping has become unstable. Row sum lumping is unstable in this case because for order 2 elements, a row sum can result in a value of zero. HRZ lumping does not display the same problems, but rather exhibits behaviour similar to the full mass matrix solution. When using both the HRZ lumping and full mass matrix, the wave-front is slightly delayed when compared with the analytical solution.

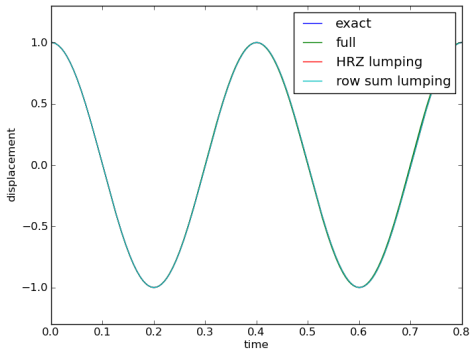


FIGURE 4.1: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the accelaraton formulation 4.30 of the Velet scheme with order 1 elements, element size $dx = 0.01$, and $c = 1$.

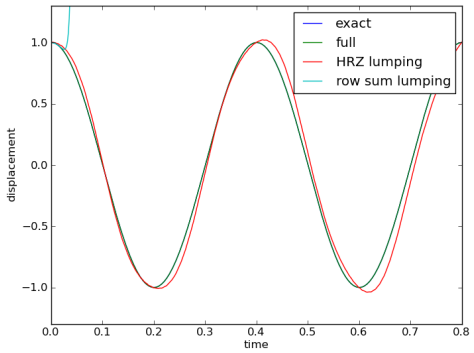


FIGURE 4.2: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the accelaraton formulation 4.30 of the Velet scheme with order 2 elements, element size 0.01, and $c = 1$.

Alternatively, one can directly solve for $u^{(n)}$ by inserting equation 4.29 into equation 4.30:

$$u^{(n)} = 2u^{(n-1)} - u^{(n-2)} + (dt \cdot c)^2 u^{(n-1)}_{,ii} \ . \tag{4.32}$$

This can also be interpreted as a PDE that must be solved at each time-step, but for the unknown $u^{(n)}$. As per equation 4.1 we set the general form coefficients to: $D = 1$; $Y = 2u^{(n-1)} - u^{(n-2)}$; and $X = -(h \cdot c)^2 u^{(n-1)}_{,i}$. For the full mass matrix, the acceleration 4.30 and displacement formulations 4.32 are identical.

The displacement solution is depicted in Figure 4.3. The domain utilised order 1 elements (for order 2, both lumping methods are unstable). The solutions for the exact and the full mass matrix approximation are almost identical while the lumping solutions, whilst identical to each other, exhibit a considerably faster wave-front propagration and a decaying amplitude.

4.4.2 Advection equation

Consider now, a second example that demonstrates the advection equation

$$u_{,t} = (v_i u)_i \ . \tag{4.33}$$

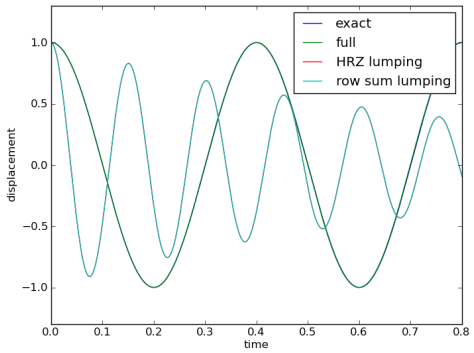


FIGURE 4.3: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the displacement formulation 4.32 of the Velet scheme with order 1 elements, element size 0.01 and $c = 1$.

where v_i is a given velocity field. To simplify this example, set $v_i = (1, 0)$ and

$$u(x,t) = \left\{ \begin{array}{ll} 1 & x_0 < t \\ 0 & x_0 \geq t \end{array} \right\}. \tag{4.34}$$

The solution scheme implemented, is the two-step Taylor-Galerkin scheme (which is in this case equivalent to SUPG): the incremental formulation is given as

$$du^{(n-\frac{1}{2})} = \frac{dt}{2}(v_i u^{(n-1)})_i \tag{4.35}$$

$$du^{(n)} = dt(v_i(u^{(n-1)} + du^{(n-\frac{1}{2})}))_i \tag{4.36}$$

$$u^{(n)} = u^{(n)} + du^{(n)} \tag{4.37}$$

This can be reformulated to calculate $u^{(n)}$ directly:

$$u^{(n-\frac{1}{2})} = u^{(n-1)} + \frac{dt}{2}(v_i u^{(n-1)})_i \tag{4.38}$$

$$u^{(n)} = u^{(n-1)} + dt(v_i u^{(n-\frac{1}{2})})_i \tag{4.39}$$

In some cases it may be possible to combine the two equations to calculate $u^{(n)}$ without the intermediate step. This approach is not discussed, because it is inflexible when a greater number of terms (e.g. a diffusion term) are added to the right hand side.

The advection problem is thus similar to the wave propagation problem, because the time step also needs to satisfy the CFL condition . For the advection problem, this takes the form

$$dt = f \cdot \frac{dx}{\|v\|}. \tag{4.40}$$

where dx is the mesh size and f is a safty factor. For this example, we again use $f = \frac{1}{6}$.

Figures 4.4 and 4.5 illustrate the four incremental formulation solutions: the true solution; the exact mass matrix; the HRZ lumping; and the row sum lumping. Observe, that for the order 1 elements case, there is little deviation from the exact solution before the wave front, whilst there is a significant degree of osciallation after the wave-front has passed. For the order 2 elements example, all of the numerical techniques fail.

Figure 4.6 depicts the results from the direct formulation of the advection problem for an order 1 mesh. Generally, the results have improved when compared with the incremental formulation. The full mass matrix still introduces some osciallation both before and after the arrival of the wave-front at the observation point. The two lumping solutions are identical, and have introduced additional smoothing to the solution. There are no oscillatory effects when using lumping for this example. In Figure 4.7 the mesh or element size has been reduced from 0.01 to 0.002 units. As predicted by the CFL condition, this significantly improves the results when lumping is applied. However, when utilising the full mass matrix, a smaller mesh size will result in post wave-front oscilations which are higher frequency and slower to decay.

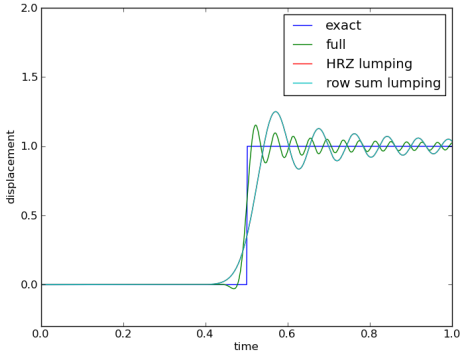


FIGURE 4.4: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the incremental formulation 4.35 of the Taylor-Galerkin scheme with order 1 elements, element size $dx = 0.01$, $v = (1, 0)$.

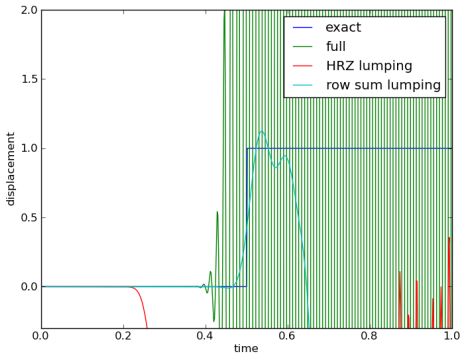


FIGURE 4.5: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the incremental formulation 4.35 of the Taylor-Galerkin scheme with order 2 elements, element size 0.01, $v = (1, 0)$.

Figure 4.8 illustrates the results when utilising elements of order 2. The full mass matrix and HRZ lumping formulations are unable to correctly model the exact solution. Only the row sum lumping was capable of producing a smooth and sensical result.

4.4.3 Sumamry

The examples in this section have demonstrated the capabilities and limitations of both HRZ and row sum lumping with comparisons to the exact and full mass matrix solutions. Wave propagation type problems that utilise lumping, produce results simular the full mass matrix at significantly lower computation cost. An accelleration based formulation, with HRZ lumping should be implemented for such problems, and can be appied to both order 1 and order 2 elements.

In transport type problems, it is essential that row sum lumping is used to achieve a smooth solution. Additionally, it is not recommended that second order elements be used in advection type problems.

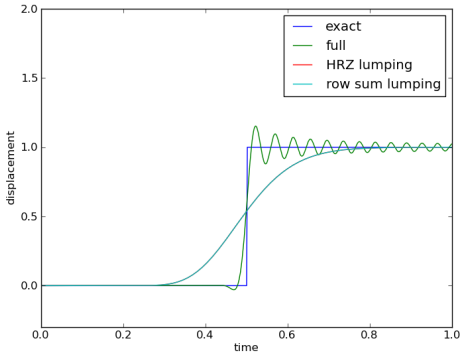


FIGURE 4.6: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the direct formulation 4.38 of the Taylor-Galerkin scheme using order 1 elements, element size $dx = 0.01$, $v = (1, 0)$.

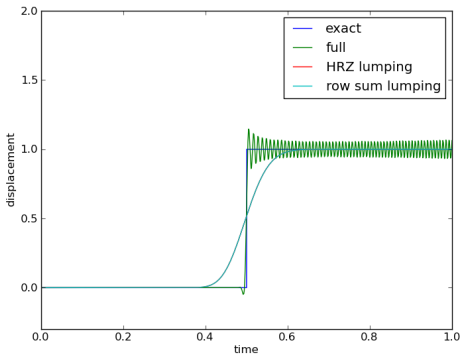


FIGURE 4.7: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the direct formulation 4.38 of the Taylor-Galerkin scheme using order 1 elements, element size $dx = 0.002$, $v = (1, 0)$.

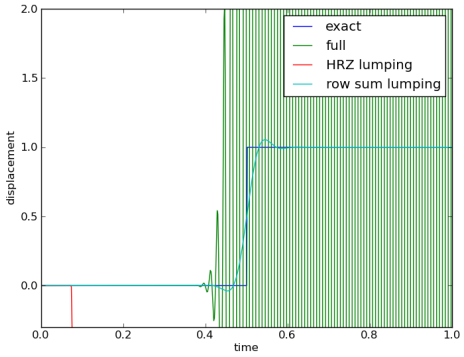


FIGURE 4.8: Amplitude at point $(\frac{1}{2}, \frac{1}{2})$ using the direct formulation 4.38 of the Taylor-Galerkin scheme using order 2 elements, element size 0.01, $v = (1, 0)$.

CHAPTER
FIVE

The `esys.pycad` Module

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 go on to build a mesh from this. The final step of generating the mesh from a `Design` uses freely available mesh generation software, such as *Gmsh*[11].

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 a `Design`, you can build meshes for arbitrarily complex 2-D and 3-D structures.

5.2 The Unit Square

The simplest geometry is the unit square. First we generate the corner points

```
from esys.pycad import *
p0=Point(0.,0.,0.)
p1=Point(1.,0.,0.)
p2=Point(1.,1.,0.)
p3=Point(0.,1.,0.)
```

which are then linked to define the edges of the square

```
l01=Line(p0,p1)
l12=Line(p1,p2)
l23=Line(p2,p3)
l30=Line(p3,p0)
```

The lines are put together to form a loop

```
c=CurveLoop(l01,l12,l23,l30)
```

The orientation of the line defining the `CurveLoop` is important. It is assumed that the surrounded area is to the left when moving along the lines from their starting points towards the end points. Moreover, the line needs to form a closed loop. We now use the `CurveLoop` to define a surface

```
s=PlaneSurface(c)
```

Note that there is a difference between the `CurveLoop`, which defines the boundary of the surface, and the actual surface `PlaneSurface`. This difference becomes clearer in the next example with a hole. Now we are ready to define the geometry which is described by an instance of the `Design` class:

```
d=Design(dim=2,element_size=0.05)
```

Here we use the two-dimensional domain with a local element size in the finite element mesh of 0.05. We then add the surface `s` to the geometry

```
d.addItems(s)
```

This will automatically import all items used to construct `s` into the `Design` `d`. Now we are ready to construct a `esys.finley` FEM mesh and then write it to the file `quad.fly`:

```
from esys.finley import MakeDomain
dom=MakeDomain(d)
dom.write("quad.fly")
```

In some cases it is useful to access the script used to generate the geometry. You can specify a specific name for the script file. In our case we use

```
d.setScriptFileName("quad.geo")
```

It is also useful to check error messages generated during the mesh generation process. *Gmsh*[11] writes messages to the file `.gmsh-errors` in your home directory. Putting everything together we get the script

```
from esys.pycad import *
from esys.pycad.gmsh import Design
from esys.finley import MakeDomain
p0=Point(0.,0.,0.)
p1=Point(1.,0.,0.)
p2=Point(1.,1.,0.)
p3=Point(0.,1.,0.)
l01=Line(p0,p1)
l12=Line(p1,p2)
l23=Line(p2,p3)
l30=Line(p3,p0)
c=CurveLoop(l01,l12,l23,l30)
s=PlaneSurface(c)
d=Design(dim=2,element_size=0.05)
d.setScriptFileName("quad.geo")
d.addItems(s)
pl1=PropertySet("sides",l01,l23)
pl2=PropertySet("top_and_bottom",l12,l30)
d.addItems(pl1, pl2)
dom=MakeDomain(d)
dom.write("quad.fly")
```

This example is included with the software in `quad.py` in the example directory.

There are three extra statements which we have not discussed yet. By default the mesh used to subdivide the boundary is not written into the mesh file mainly to reduce the size of the data file. One needs to explicitly add the lines to the `Design` which should be present in the mesh data. Here we additionally labeled the lines on the top and the bottom with the name "top_and_bottom" and the lines on the left and right hand side with the name "sides" using `PropertySet` objects. The labeling is convenient when using tagging, see Chapter 3.

If you have *Gmsh*[11] installed you can run the example and view the geometry and mesh with:

```
run-escript quad.py
gmsh quad.geo
gmsh quad.msh
```

See Figure 5.1 for a result.

In most cases it is best practice to generate the mesh and solve the mathematical model in two separate scripts. In our example you can read the `esys.finley` mesh into your simulation code[1] using

```
from finley import ReadMesh
mesh=ReadMesh("quad.fly")
```

Note that the underlying mesh generation software will not accept all the geometries you can create. For example, `esys.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*[11] will fail to create a mesh for it.

[1] *Gmsh*[11] files can be directly read using `ReadGmsh`, see Chapter 7

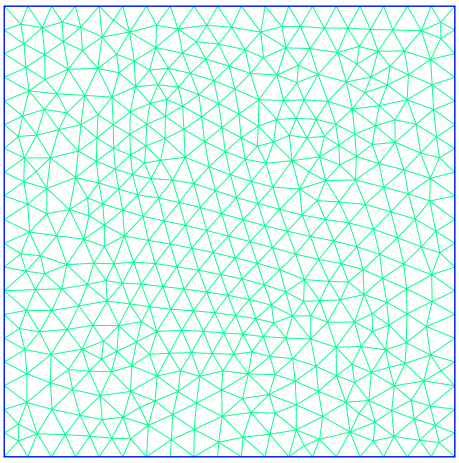


FIGURE 5.1: Quadrilateral with mesh of triangles

5.3 Holes

The example included below shows how to use `esys.pycad` to create a 2-D mesh in the shape of a trapezoid with a cut-out area as in Figure 5.2.

```
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)
```

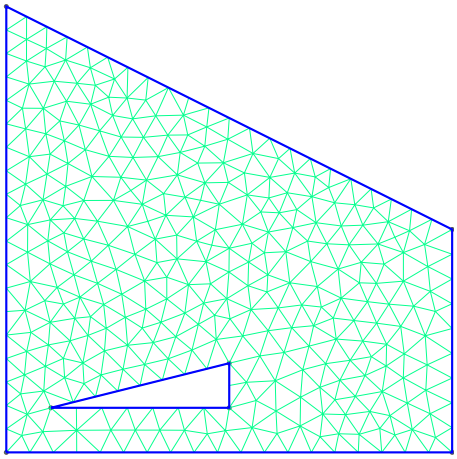


FIGURE 5.2: Trapezoid with triangular hole

```
# write mesh to a finley file:
domain.write("trapezoid.fly")
```

This example is included with the software in `trapezoid.py` in the example directory.

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 define any number of lines when creating a `CurveLoop`, but the end of one line must be identical to the start of the next.

5.4 A 3D example

In this section we discuss the definition of 3D geometries. As an example consider the unit cube as shown in Figure 5.3. First we generate the vertices of the cube:

```
from esys.pycad import *
p0=Point(0.,0.,0.)
p1=Point(1.,0.,0.)
p2=Point(0.,1.,0.)
p3=Point(1.,1.,0.)
p4=Point(0.,0.,1.)
p5=Point(1.,0.,1.)
p6=Point(0.,1.,1.)
p7=Point(1.,1.,1.)
```

We connect the points to form the bottom and top surfaces of the cube:

```
l01=Line(p0,p1)
l13=Line(p1,p3)
l32=Line(p3,p2)
l20=Line(p2,p0)
bottom=PlaneSurface(-CurveLoop(l01,l13,l32,l20))
```

Similar to the definition of a `CurvedLoop` the orientation of the surfaces in a `SurfaceLoop` is relevant. In fact, the surface normal direction defined by the right-hand rule needs to point outwards as indicated by the surface normals in Figure 5.3. As the `bottom` face is directed upwards it is inserted with the minus sign into the `SurfaceLoop` in order to adjust the orientation of the surface. Similarly we set

```
l45=Line(p4,p5)
l57=Line(p5,p7)
l76=Line(p7,p6)
l64=Line(p6,p4)
top=PlaneSurface(CurveLoop(l45,l57,l76,l64))
```

To form the front face we introduce the two additional lines connecting the left and right front points of the `top` and `bottom` face:

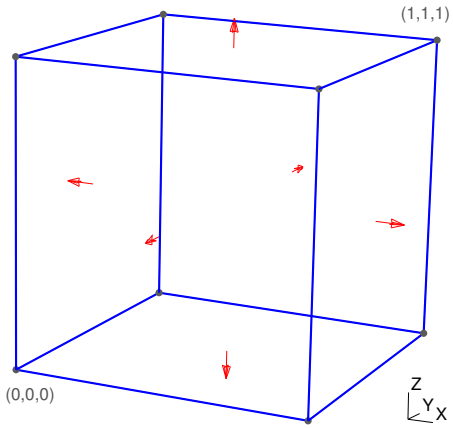


FIGURE 5.3: Three dimensional block

```
l15=Line(p1,p5)
l40=Line(p4,p0)
```

To form the front face we encounter the problem as the line `l45` used to define the `top` face is pointing the wrong direction. In `esys.pycad` you can reversing direction of an object by changing its sign. So we write `-l45` to indicate that the direction is to be reversed. With this notation we can write

```
front=PlaneSurface(CurveLoop(l01,l15,-l45,l40))
```

Keep in mind that if you use `Line(p4,p5)` instead of `-l45` both objects are treated as different although connecting the same points with a straight line in the same direction. The resulting geometry would include an opening along the `p4`–`p5` connection. This will lead to an inconsistent mesh and may result in a failure of the volumetric mesh generator. Similarly we can define the other sides of the cube:

```
l37=Line(p3,p7)
l62=Line(p6,p2)
back=PlaneSurface(CurveLoop(l32,-l62,-l76,-l37))
left=PlaneSurface(CurveLoop(-l40,-l64,l62,l20))
right=PlaneSurface(CurveLoop(-l15,l13,l37,-l57))
```

We can now put the six surfaces together to form a `SurfaceLoop` defining the boundary of the volume of the cube:

```
sl=SurfaceLoop(top,bottom,front,back,left,right)
v=Volume(sl)
```

As in the 2D case, the `Design` class is used to define the geometry:

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

des=Design(dim=3, element_size = 0.1, keep_files=True)
des.setScriptFileName("brick.geo")
des.addItems(v, top, bottom, back, front, left, right)

dom=MakeDomain(des)
dom.write("brick.fly")
```

Note that the `esys.finley` mesh file `brick.fly` will contain the triangles used to define the surfaces as they are added to the `Design`. The example script of the cube is included with the software in `brick.py` in the example directory.

5.5 Alternative File Formats

`esys.pycad` supports other file formats including I-DEAS universal file, VRML, Nastran and STL. The following example shows how to generate the STL file `brick.stl`:

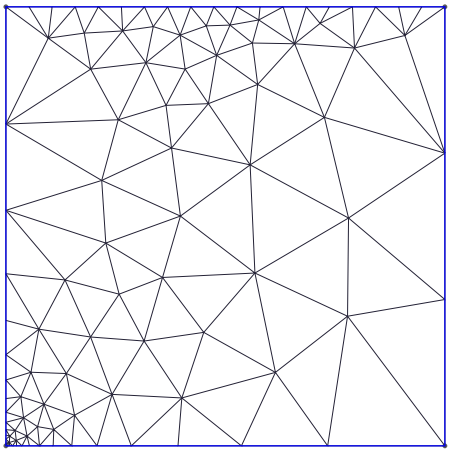


FIGURE 5.4: Local refinement at the origin by `local_scale=0.01` with `element_size=0.3` and number of elements on the top set to 10

```
from esys.pycad.gmsh import Design

des=Design(dim=3, element_size = 0.1, keep_files=True)
des.addItems(v, top, bottom, back, front, left , right)

des.setFileFormat(des.STL)
des.setMeshFileName("brick.stl")
des.generate()
```

The example script of the cube is included with the software in `brick_stl.py` in the example directory.

5.6 Element Sizes

The element size used globally is defined by the `element_size` argument of the `Design`. The mesh generator will try to use this mesh size everywhere in the geometry. In some cases it can be desirable to use a finer mesh locally. A local refinement can be defined at each `Point`:

```
p0=Point(0., 0., 0., local_scale=0.01)
```

Here the mesh generator will create a mesh with an element size which is by the factor `0.01` times smaller than the global mesh size `element_size=0.3`, see Figure 5.4. The point where a refinement is defined must be a point on a curve used to define the geometry.

Alternatively, one can define a mesh size along a curve by defining the number of elements to be used to subdivide the curve. For instance, to use 20 elements on line `l23`:

```
l23=Line(p2, p3)
l23.setElementDistribution(20)
```

Setting the number of elements on a curve overwrites the global mesh size `element_size`. The result is shown in Figure 5.4.

5.7 `esys.pycad` Classes

5.7.1 Primitives

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

class Point(x=0.,y=0.,z=0.[,local_scale=1.])

creates a point at the given coordinates with local characteristic length `local_scale`

class CurveLoop(list)
creates a closed curve from a `list` of `Line`, `Arc`, `Spline`, `BSpline`, `BezierSpline` objects.

class SurfaceLoop(list)
creates a loop of `PlaneSurface` or `RuledSurface`, which defines the shell of a volume.

5.7.1.1 Lines

class Line(point1, point2)
creates a line between two points.

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on the line. If set, it overwrites the local length setting which would be applied. The progression factor `progression` defines the change of element size between neighboured elements. If `createBump` is set progression is applied towards the centre of the line.

resetElementDistribution()
removes a previously set element distribution from the line.

getElementDistribution()
returns the element distribution as a tuple of number of elements, progression factor and bump flag. If no element distribution is set None is returned.

5.7.1.2 Splines

class Spline(point0, point1, ...)
A spline curve defined by a list of points `point0`, `point1`, ...

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on the spline. If set, it overwrites the local length setting which would be applied. The progression factor `progression` defines the change of element size between neighboured elements. If `createBump` is set progression is applied towards the centre of the spline.

resetElementDistribution()
removes a previously set element distribution from the spline.

getElementDistribution()
returns the element distribution as a tuple of number of elements, progression factor and bump flag. If no element distribution is set None is returned.

5.7.1.3 BSplines

class BSpline(point0, point1, ...)
A B-spline curve defined by a list of points `point0`, `point1`, ...

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on the curve. If set, it overwrites the local length setting which would be applied. The progression factor `progression` defines the change of element size between neighboured elements. If `createBump` is set progression is applied towards the centre of the curve.

resetElementDistribution()

removes a previously set element distribution from the curve.

getElementDistribution()
returns the element distribution as a tuple of number of elements, progression factor and bump flag. If no element distribution is set None is returned.

5.7.1.4 Bezier Curves

class BezierCurve(point0, point1, ...)
A Bezier spline curve defined by a list of points `point0`, `point1`, ...

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on the curve. If set, it overwrites the local length setting which would be applied. The progression factor `progression` defines the change of element size between neighboured elements. If `createBump` is set progression is applied towards the centre of the curve.

resetElementDistribution()
removes a previously set element distribution from the curve.

getElementDistribution()
returns the element distribution as a tuple of number of elements, progression factor and bump flag. If no element distribution is set None is returned.

5.7.1.5 Arcs

class Arc(centre_point, start_point, end_point)
creates an arc by specifying a centre for a circle and start and end points. An arc may subtend an angle of at most π radians.

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on the arc. If set, it overwrites the local length setting which would be applied. The progression factor `progression` defines the change of element size between neighboured elements. If `createBump` is set progression is applied towards the centre of the arc.

resetElementDistribution()
removes a previously set element distribution from the arc.

getElementDistribution()
returns the element distribution as a tuple of number of elements, progression factor and bump flag. If no element distribution is set None is returned.

5.7.1.6 Plane surfaces

class PlaneSurface(loop, [holes=[list]])
creates a plane surface from a `CurveLoop`, which may have one or more holes described by a `list` of `CurveLoop` objects.

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on all lines.

setRecombination([max_deviation=45 * `DEG`])

the mesh generator will try to recombine triangular elements into quadrilateral elements. `max_deviation` (in radians) defines the maximum deviation of any angle in the quadrilaterals from the right angle. Set `max_deviation` =`None` to remove recombination.

setTransfiniteMeshing([orientation="Left"])
applies 2D transfinite meshing to the surface. `orientation` defines the orientation of triangles. Allowed values are ``Left'', ``Right'' and ``Alternate''. The boundary of the surface must be defined by three or four lines and an element distribution must be defined on all faces where opposite faces use the same element distribution. No holes must be present.

5.7.1.7 Ruled Surfaces

class RuledSurface(list)
creates a surface that can be interpolated using transfinite interpolation. `list` gives a list of three or four lines defining the boundary of the surface.

setRecombination([max_deviation=45 * `DEG`])
the mesh generator will try to recombine triangular elements into quadrilateral elements. `max_deviation` (in radians) defines the maximum deviation of any angle in the quadrilaterals from the right angle. Set `max_deviation` =`None` to remove recombination.

setTransfiniteMeshing([orientation="Left"])
applies 2D transfinite meshing to the surface. `orientation` defines the orientation of triangles. Allowed values are ``Left'', ``Right'' and ``Alternate''. The boundary of the surface must be defined by three or four lines and an element distribution must be defined on all faces where opposite faces use the same element distribution. No holes must be present.

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on all lines.

5.7.1.8 Volumes

class Volume(loop, [holes=[list]])
creates a volume given a `SurfaceLoop`, which may have one or more holes define by the list of `SurfaceLoop`.

setElementDistribution(n[,progression=1[,createBump=*False*]])
defines the number of elements on all lines.

setRecombination([max_deviation=45 * `DEG`])
the mesh generator will try to recombine triangular elements into quadrilateral elements. These meshes are then used to generate the volume mesh if possible. Together with transfinite meshing one can construct rectangular meshes. `max_deviation` (in radians) defines the maximum deviation of any angle in the quadrilaterals from the right angle. Set `max_deviation` =`None` to remove recombination.

setTransfiniteMeshing([orientation="Left"])
applies transfinite meshing to the volume and all surfaces (if `orientation` is not equal to `None`). `orientation` defines the orientation of triangles. Allowed values are ``Left'', ``Right'' and ``Alternate''. The boundary of the surface must be defined by three or four lines and an element distribution must be defined on all faces where opposite faces use the same element distribution. If `orientation` is equal to `None` transfinite meshing is not switched on for the surfaces but needs to be set by the user. No holes must be present. **Warning: The functionality of transfinite meshing without recombination is not entirely clear in *Gmsh*[11]. So please apply this method with care.**

5.7.2 Transformations

Sometimes it is convenient to create an object and then make copies at different orientations or in different sizes. This can be achieved by applying transformations which are used to move geometrical objects in the 3-dimensional space and to resize them.

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

class Rotation([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 `numpy` object of shape $(3,)$. `axis` does not have to be normalised but must have positive length. The right-hand rule [26] applies.

class Dilation([factor=1., [centre=[0,0,0]]])
defines a dilation by the expansion/contraction `factor` with `centre` as the dilation centre. `centre` can be any object that can be converted into a `numpy` 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 `numpy` object of shape $(3,)$. `normal` does not have to be normalised 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.

5.7.3 Properties

If you are building a larger geometry you may find it convenient to create it in smaller pieces and then assemble them. 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 which share the same material properties or to mark portions of the boundary. For efficiency, the `Design` class assigns an 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

5.8 Interface to the mesh generation software

The class and methods described here provide an interface to the mesh generation software, which is currently *Gmsh*[11]. 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]]]])
describes the geometry defined by primitives to be meshed. `dim` specifies the spatial dimension, while `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 are kept, otherwise they are removed when the instance of the class is deleted.

GMSH
gmsh file format [11]

IDEAS
I-DEAS universal file format [15]

VRML
VRML file format, [35]

STL
STL file format [31]

NASTRAN
NASTRAN bulk data format [21]

MEDIT
Medit file format [17]

CGNS
CGNS file format [3]

PLOT3D
Plot3D file format [25]

DIFFPACK
Diffpack 3D file format [8]

DELAUNAY
the Delaunay triangulator, see *Gmsh*[11] and [29]

MESHADAPT
the gmsh triangulator, see *Gmsh*[11]

FRONTAL
the NETGEN [9] triangulator

generate()
generates the mesh file. The data are written to the file `Design.getMeshFileName`.

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])
sets 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.

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, *False* otherwise.

setScriptFileName([name=None])
sets the file name 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 mesh file. If no name is given a name is generated. The format is set by `Design.setFileFormat`.

getMeshFileName()
returns the name of the mesh file.

addItems(*items)
adds the tuple of `items`. An item can be any primitive or a `PropertySet`. *Warning: If a `PropertySet` is added which includes an object that is not part of a `PropertySet`, it may not be considered in the meshing.*

getItems()
returns a list of the items.

clearItems()
resets the items in this design.

getMeshHandler()
returns a handle to the mesh. Calling 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 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 a string.

setOptions([optimize_quality=*True* [, smoothing=1 [, curvature_based_element_size=*False*
[, algorithm2D=`Design.MESHADAPT` [, algorithm3D=`Design.FRONTAL`
[, generate_hexahedra=False]]]]]])
sets options for the mesh generator. `algorithm2D` sets the 2D meshing algorithm to be used. The algorithm needs to be `Design.DELAUNAY`, `Design.FRONTAL`, or `Design.MESHADAPT`. By default `Design.MESHADAPT` is used. `algorithm3D` sets the 3D meshing algorithm to be used. The algorithm needs to be `Design.DELAUNAY` or `Design.FRONTAL`. By default `Design.FRONTAL` 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. `curvature_based_element_size` =*True* switches on curvature based definition of element size. `generate_hexahedra` =*True* switches on the usage of quadrilateral or hexahedral elements.

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

setFileFormat([format=`Design.GMSH`])
sets the file format. `format` must be one of the values:
`Design.GMSH`
`Design.IDEAS`
`Design.VRML`
`Design.STL`
`Design.NASTRAN`
`Design.MEDIT`
`Design.CGNS`
`Design.PLOT3D`
`Design.DIFFPACK`.

getFileFormat()
returns the file format.

CHAPTER
SIX

Models

The following sections give a brief overview of the model classes and their corresponding methods.

6.1 The Stokes Problem

In this section we discuss how to solve the Stokes problem. We want to calculate the velocity field v and pressure p of an incompressible fluid. They are given as the solution of the Stokes problem

$$-\left(\eta(v_{i,j}+v_{j,i})\right)_{,j}+p_{,i}=f_i-\sigma_{ij,j} \tag{6.1}$$

where f_i defines an internal force and σ_{ij} is an initial stress. The viscosity η may weakly depend on pressure and velocity. If relevant we will use the notation $\eta(v,p)$ to express this dependency.

We assume an incompressible medium:

$$-v_{i,i}=0 \tag{6.2}$$

Natural boundary conditions are taken in the form

$$\left(\eta(v_{i,j}+v_{j,i})\right)n_j-n_ip=s_i-\alpha\cdot n_in_jv_j+\sigma_{ij}n_j \tag{6.3}$$

which can be overwritten by constraints of the form

$$v_i(x)=v_i^D(x) \tag{6.4}$$

at some locations x at the boundary of the domain. s_i defines a normal stress and $\alpha\geq 0$ the spring constant for restoring normal force. The index i may depend on the location x on the boundary. v^D is a given function on the domain.

6.1.1 Solution Method

If we assume that η is independent from the velocity and pressure, equations 6.1 and 6.2 can be written in the block form

$$\begin{bmatrix} A & B^* \\ B & 0 \end{bmatrix}\begin{bmatrix} v \\ p \end{bmatrix}=\begin{bmatrix} G \\ 0 \end{bmatrix} \tag{6.5}$$

where A is a coercive, self-adjoint linear operator in a suitable Hilbert space, B is the $(-1)\cdot$ divergence operator and B^* is the adjoint operator (=gradient operator). For more details on the mathematics see references [1, 2].

If v_0 and p_0 are given initial guesses for velocity and pressure we calculate a correction dv for the velocity by solving the first equation of Equation (6.5)

$$Adv_1=G-Av_0-B^*p_0 \tag{6.6}$$

We then insert the new approximation $v_1 = v_0 + dv_1$ to calculate a correction dp_2 for the pressure and an additional correction dv_2 for the velocity by solving

$$\begin{aligned} BA^{-1}B^* dp_2 &= Bv_1 \\ Adv_2 &= B^* dp_2 \end{aligned} \tag{6.7}$$

The new velocity and pressure are then given by $v_2 = v_1 - dv_2$ and $p_2 = p_0 + dp_2$ which will fulfill the block system 6.5. This solution strategy is called the Uzawa scheme.

There is a problem with this scheme: in practice we will use an iterative scheme to solve any problem for operator A. So we will be unable to calculate the operator $BA^{-1}B^*$ required for dp_2 explicitly. In fact, we need to use another iterative scheme to solve the first equation in 6.7 where in each iteration step an iterative solver for A is applied. Another issue is the fact that the viscosity η may depend on velocity or pressure and so we need to iterate over the three equations 6.6 and 6.7.

In the following we will use the two norms

$$\|v\|_1^2 = \int_\Omega v_{j,k} v_{j,k} \, dx \text{ and } \|p\|_0^2 = \int_\Omega p^2 \, dx. \tag{6.8}$$

for velocity v and pressure p. The iteration is terminated if the stopping criterion

$$\max(\|Bv_1\|_0, \|v_2 - v_0\|_1) \leq \tau \cdot \|v_2\|_1 \tag{6.9}$$

for a given tolerance $0 < \tau < 1$ is met. Notice that because of the first equation of 6.7 we have that $\|Bv_1\|_0$ equals the norm of $BA^{-1}B^*dp_2$ and consequently provides a norm for the pressure correction.

We want to optimize the tolerance choice for solving 6.6 and 6.7. To do this we write the iteration scheme as a fixed point problem. Here we consider the errors produced by the iterative solvers being used. From Equation (6.6) we have

$$v_1 = e_1 + v_0 + A^{-1}(G - Av_0 - B^* p_0) \tag{6.10}$$

where e_1 is the error when solving 6.6. We will use a sparse matrix solver so we have not full control on the norm $\|.\|_s$ used in the stopping criterion for this equation. In fact we will have a stopping criterion of the form

$$\|Ae_1\|_s = \|G - Av_1 - B^* p_0\|_s \leq \tau_1 \|G - Av_0 - B^* p_0\|_s \tag{6.11}$$

where τ_1 is the tolerance which we need to choose. This translates into the condition

$$\|e_1\|_1 \leq K\tau_1 \|dv_1 - e_1\|_1 \tag{6.12}$$

The constant K represents some uncertainty combining a variety of unknown factors such as the norm being used and the condition number of the stiffness matrix. From the first equation of 6.7 we have

$$p_2 = p_0 + (BA^{-1}B^*)^{-1}(e_2 + Bv_1) \tag{6.13}$$

where e_2 represents the error when solving 6.7. We use an iterative preconditioned conjugate gradient method (PCG) with iteration operator $BA^{-1}B^*$ using the $\|.\|_0$ norm. As suitable preconditioner for the iteration operator we use $\frac{1}{\eta}$ [30], i.e. the evaluation of the preconditioner P for a given pressure increment q is the solution of

$$\frac{1}{\eta}(Pq) = q \, . \tag{6.14}$$

Note that in each evaluation of the iteration operator $q = BA^{-1}B^*s$ one needs to solve the problem

$$Aw = B^* s \tag{6.15}$$

with sufficient accuracy to return $q = Bw$. We assume that the desired tolerance is sufficiently small, for instance one can take τ_2^2 where τ_2 is the tolerance for 6.7.

In an implementation we use the fact that the residual r is given as

$$r = B(v_1 - A^{-1}B^* dp) = B(v_1 - A^{-1}B^* dp) = B(v_1 - dv_2) = Bv_2 \tag{6.16}$$

In particular we have $e_2 = Bv_2$. So the residual r is represented by the updated velocity $v_2 = v_1 - dv_2$. In practice, if one uses the velocity to represent the residual r there is no need to recover dv_2 in 6.7 after dp_2 has been calculated. In PCG the iteration is terminated if

$$\|P^{\frac{1}{2}} Bv_2\|_0 \leq \tau_2 \|P^{\frac{1}{2}} Bv_1\|_0 \tag{6.17}$$

where τ_2 is the given tolerance. This translates into

$$\|e_2\|_0 = \|Bv_2\|_0 \leq M\tau_2 \|Bv_1\|_0 \tag{6.18}$$

where M is taking care of the fact that $P^{\frac{1}{2}}$ is dropped.

As we assume that there is no significant error from solving with the operator A we have

$$v_2 = v_1 - dv_2 = v_1 - A^{-1}B^* dp \tag{6.19}$$

Combining the equations 6.10, 6.13 and 6.19 and setting the errors to zero we can write the solution process as a fix point problem

$$v = \Phi(v, p) \text{ and } p = \Psi(u, p) \tag{6.20}$$

with suitable functions $\Phi(v, p)$ and $\Psi(v, p)$ representing the iteration operator without errors. In fact, for a linear problem, Φ and Ψ are constant. With this notation we can write the update step in the form $p_2 = \delta p + \Psi(v_0, p_0)$ and $v_2 = \delta v + \Phi(v_0, p_0)$ where the total error δp and δv are given as

$$\begin{array}{rcl} \delta p & = & (BA^{-1}B^*)^{-1}(e_2 + Be_1) \\ \delta v & = & e_1 - A^{-1}B^* \delta p \; . \end{array} \tag{6.21}$$

Notice that $B\delta v = -e_2 = -Bv_2$. Our task is now to choose the tolerances τ_1 and τ_2 such that the global errors δp and δv do not stop the convergence of the iteration process.

To measure convergence we use

$$\epsilon = \max(\|v_2 - v\|_1, \|BA^{-1}B^*(p_2 - p)\|_0) \tag{6.22}$$

In practice using the fact that $BA^{-1}B^*(p_2 - p_0) = Bv_1$ and assuming that v_2 gives a better approximation to the true v than v_0 we will use the estimate

$$\epsilon = \max(\|v_2 - v_0\|_1, \|Bv_1\|_0) \tag{6.23}$$

to estimate the progress of the iteration step after the step is completed. Note that the estimate of ϵ is used in the stopping criterion 6.9. If χ^- is the convergence rate assuming exact calculations, i.e. $e_1 = 0$ and $e_2 = 0$, we are expecting to maintain $\epsilon \leq \chi^- \cdot \epsilon^-$. For the pressure increment we get:

$$\begin{array}{rcl} \|BA^{-1}B^*(p_2 - p)\|_0 & \leq & \|BA^{-1}B^*(p_2 - \delta p - p)\|_0 + \|BA^{-1}B^* \delta p\|_0 \\ & = & \chi^- \cdot \epsilon^- + \|e_2 + Be_1\|_0 \\ & \approx & \chi^- \cdot \epsilon^- + \|e_2\|_0 \\ & \leq & \chi^- \cdot \epsilon^- + M\tau_2 \|Bv_1\|_0 \end{array} \tag{6.24}$$

So we choose the value for τ_2 from

$$M\tau_2 \|Bv_1\|_0 \leq (\chi^-)^2 \epsilon^- \tag{6.25}$$

in order to make the perturbation for the termination of the pressure iteration a second order effect. We use a similar argument for the velocity:

$$\begin{array}{rcl} \|v_2 - v\|_1 & \leq & \|v_2 - \delta v - v\|_1 + \|\delta v\|_1 \\ & \leq & \chi^- \cdot \epsilon^- + \|e_1 - A^{-1}B^* \delta p\|_1 \\ & \approx & \chi^- \cdot \epsilon^- + \|e_1\|_1 \\ & \leq & \chi^- \cdot \epsilon^- + K\tau_1 \|dv_1 - e_1\|_1 \\ & \leq & (1 + K\tau_1)\chi^- \cdot \epsilon^- \end{array} \tag{6.26}$$

So we choose the value for τ_1 from

$$K\tau_1 \leq \chi^- \tag{6.27}$$

Assuming we have estimates for M and K[1] we can use 6.27 and 6.25 to get appropriate values for the tolerances. After the step has been completed we can calculate a new convergence rate $\chi = \frac{\epsilon}{\epsilon^-}$. For partial reasons we restrict χ to be less or equal a given maximum value $\chi_{max} \leq 1$. If we see $\chi \leq \chi^-(1+\chi^-)$ our choices for the tolerances were suitable. Otherwise, we need to adjust the values for K and M. From the estimates 6.24 and 6.26 we establish

$$\chi \leq (1 + \max(M\frac{\tau_2\|Bv_1\|_0}{\chi^-\epsilon^-}, K\tau_1)) \cdot \chi^- \tag{6.28}$$

If we assume that this inequality would be an equation if we would have chosen the right values M^+ and K^+ then we get

$$\chi = (1 + \max(M^+\frac{\chi^-}{M}, K^+\frac{\chi^-}{K})) \cdot \chi^- \tag{6.29}$$

From this equation we see if our choice for K was not good enough. In this case we can calculate a new value

$$K^+ = \frac{\chi - \chi^-}{(\chi^-)^2}K \tag{6.30}$$

In practice we will use

$$K^+ = \max(\frac{\chi - \chi^-}{(\chi^-)^2}K, \frac{1}{2}K, 1) \tag{6.31}$$

where the second term is used to reduce a potential overestimate of K. The same identity is used for to update M. The updated M^+ and K^+ are then use in the next iteration step to control the tolerances.

In some cases one can observe that there is a significant change in the velocity but the new velocity v_1 has still a small divergence, i.e. we have $\|Bv_1\|_0 \ll \|v_1 - v_0\|_1$. In this case we will get a small pressure increment and consequently only very small changes to the velocity as a result of the second update step which therefore can be skipped and we can directly repeat the first update step until the increment in velocity becomes significant relative to its divergence. In practice we will ignore the second half of the iteration step as long as

$$\|Bv_1\|_0 \leq \theta \cdot \|v_1 - v_0\| \tag{6.32}$$

where $0 < \theta < 1$ is a given factor. In this case we will also check the stopping criterion with $v_1 \to v_2$ but we will not correct M in this case.

Starting from an initial guess v_0 and p_0 for velocity and pressure the solution procedure is implemented as follows:

1. calculate viscosity $\eta(v_0, p)_0$ and assemble operator A from η
2. calculate the tolerance τ_1 from Equation (6.27)
3. solve Equation (6.6) for dv_1 with tolerance τ_1
4. update $v_1 = v_0 + dv_1$
5. if Bv_1 is large (see 6.32):
   (a) calculate the tolerance τ_2 from 6.25
   (b) solve 6.7 for dp_2 and v_2 with tolerance τ_2
   (c) update $p_2 \leftarrow p_0 + dp_2$
6. else:
   - update $p_2 \leftarrow p$ and $v_2 \leftarrow v_1$
7. calculate convergence measure ϵ and convergence rate χ
8. if stopping criterion 6.9 holds:
   - return v_2 and p_2
9. else:
   (a) update M and K
   (b) goto step 1 with $v_0 \leftarrow v_2$ and $p_0 \leftarrow p_2$.

[1] if no estimates are available, we use the value 1

6.1.2 Functions

class StokesProblemCartesian(domain)

opens the Stokes problem on the `Domain` domain. The domain needs to support LBB compliant elements for the Stokes problem, see [12] for details. For instance one can use second order polynomials for velocity and first order polynomials for the pressure on the same element. Alternatively, one can use macro elements using linear polynomials for both pressure and velocity with a subdivided element for the velocity. Typically, the macro element is more cost effective. The fact that pressure and velocity are represented in different ways is expressed by

```
velocity=Vector(0.0, Solution(mesh))
pressure=Scalar(0.0, ReducedSolution(mesh))
```

initialize([f=Data(), [fixed_u_mask=Data(), [eta=1,[surface_stress=Data(), [stress=Data()],[restoration_factor=0]]]]])

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 components where the velocity is fixed are set by the values of `fixed_u_mask`. `restoration_factor` defines the restoring force factor α. The method will try to cast the given values to appropriate `Data` class objects.

solve(v,p [, max_iter=100 [, verbose=False [, usePCG=True]]])

solves the problem and returns approximations for velocity and pressure. The arguments `v` and `p` define initial guesses. `v` must have function space `Solution(domain)` and `p` must have function space `ReducedSolution(domain)`. The values of `v` marked by `fixed_u_mask` remain unchanged. If `usePCG` is set to *True* then the preconditioned conjugate gradient method (PCG) scheme is used. Otherwise the problem is solved with the generalized minimal residual method (GMRES). In most cases the PCG scheme is more efficient. `max_iter` defines the maximum number of iteration steps. If `verbose` is set to *True* information on the progress of of the solver is printed.

setTolerance([tolerance=1.e-4])

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 tolerance is set to 0.

getAbsoluteTolerance()

returns the current absolute tolerance.

getSolverOptionsVelocity()

returns the solver options used to solve Equation (6.6) and Equation (6.15)) for velocity.

getSolverOptionsPressure()

returns the solver options used to solve the preconditioner Equation (6.14) for pressure.

getSolverOptionsDiv()

sets the solver options for solving the equation to project the divergence of the velocity onto the function space of pressure.

setStokesEquation([f=None, [fixed_u_mask=None, [eta=None,[surface_stress=None, [stress=None],[restoration_factor=None]]]]])

assigns new values to the model parameters, see method `initialize` for description of the parameter list. In contrast to `initialize` only values given in the argument list are set. Typically this method is called to update parameters such as viscosity η within a time integration scheme after the problem has been set up by an initial call of method `initialize`.

updateStokesEquation(v, p)

this method is called by the solver to allow for updating the model parameter during the iteration process for incompressibility. In order to implement a non-linear dependence of model parameters such as viscosity η from the current velocity `v` or pressure field `p` this function can be overwritten in the following way:

```
class MyStokesProblem(StokesProblemCartesian):
   def updateStokesEquation(self, v, p):
       my_eta=<eta derived from v and p>
       self.setStokesEquation(eta=my_eta)
```

Note that `setStokesEquation` to update the model. *Warning: It is not guaranteed that the iteration converges if model parameters are altered.*

6.1.3 Example: Lid-driven Cavity

The following script `lid_driven_cavity.py` which is available in the example directory illustrates the usage of the `StokesProblemCartesian` class to solve the lid-driven cavity problem:

```
from esys.escript import *
from esys.finley import Rectangle
from esys.weipa import saveVTK
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.vtu", velocity=v, pressure=p)
```

6.2 Darcy Flux

We want to calculate the velocity u and pressure p on a domain Ω solving the Darcy flux problem

$$\begin{aligned} u_i + \kappa_{ij} p_{,j} &= g_i \\ u_{k,k} &= f \end{aligned} \tag{6.33}$$

with the boundary conditions

$$\begin{aligned} u_i \, n_i = u_i^N \, n_i \quad &\text{on} \quad \Gamma_N \\ p = p^D \quad &\text{on} \quad \Gamma_D \end{aligned} \tag{6.34}$$

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 permeability. 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 which are independent from the location in Ω such that

$$\alpha_0 \, x_i x_i \leq \kappa_{ij} x_i x_j \leq \alpha_1 \, x_i x_i \tag{6.35}$$

for all x_i.

6.2.1 Solution Method

Unfortunate equation 6.33 can not solved directly in an easy way and requires mixed FEM. We consider a few options to solve equation 6.33

6.2.1.1 Evaluation

The first equation of equation 6.33 is inserted into the second one:

$$-(\kappa_{ij}p_{,j})_{,i} = f - (g_i)_{,i} \tag{6.36}$$

with boundary conditions

$$\begin{aligned} \kappa_{ij}p_{,j}\ n_i = (g_i - u_i^N)\ n_i \quad &\text{on} \quad \Gamma_N \\ p = p^D \quad &\text{on} \quad \Gamma_D \end{aligned} \tag{6.37}$$

Then the flux field is recovered by directly setting

$$u_j = g_j - \kappa_{ij}p_{,j} \tag{6.38}$$

This simple recovery process will not ensure that the (numerically) calculated flux meets the boundary conditions for flux or the incompressibility condition. However this is a very fast way of calculating the flux.

6.2.1.2 Global Postprocessing

An improved flux recovery can be achieved by solving a modified version of equation 6.38 adding the the gradient of the divergence of the flux:

$$\kappa_{ij}^{-1}u_j - (\lambda \cdot u_{k,k})_{,i} = \kappa_{ij}^{-1}g_j - p_{,i} - (\lambda \cdot f)_{,i} \tag{6.39}$$

where

$$\lambda = \omega \cdot |\kappa^{-1}| \cdot vol(\Omega)^{1/d} \cdot h \tag{6.40}$$

with a non-negative factor ω, d is the spatial dimension and h is the local element size.

$$\begin{aligned} u_i\ n_i = u_i^N\ n_i \quad &\text{on} \quad \Gamma_N \\ u_{k,k} = f \quad &\text{on} \quad \Gamma_D \end{aligned} \tag{6.41}$$

Notice that the second condition is a natural boundary condition. Global post-processing is more expense than direct pressure evaluation however the flux is more accurate and asymptotic incompressibility for mesh size towards zero can be shown, if $\omega > 0$.

6.2.2 Functions

class DarcyFlow(domain, [w=1., [solver=`DarcyFlow.EVAL`, [useReduced=*True*, [verbose=*True*]]]])

opens the Darcy flux problem on the `Domain` domain. Reduced approximations for pressure and flux are used if `useReduced` is set. Argument `solver` defines the solver method. If `verbose` is set some information are printed. `w` defines the weighting factor ω for global post-processing of the flux (see equation 6.40.)

EVAL
flux is calculated directly from pressure evaluation, see section 6.2.1.1.

SMOOTH
solver using global post-processing of flux with weighting factor $\omega = 0$, see section 6.2.1.2.

POST
solver using global post-processing of flux, see section 6.2.1.2.

setValue([f=None, [g=None, [location_of_fixed_pressure=None, [location_of_fixed_flux=None, [permeability=None]]]]])

assigns values to the model parameters. Values can be assigned using various calls – in particular in a time dependent problem only values that change over time need to be reset. The permeability can be defined as a scalar (isotropic), or a symmetric matrix (anisotropic). `f` and `g` are the corresponding parameters in 6.33. The locations and components where the flux is prescribed are set by positive values in `location_of_fixed_flux`. The locations where the pressure is prescribed are set by by positive values of `location_of_fixed_pressure`. The values of the pressure and flux are defined by the initial guess. Notice that at any point on the boundary of the domain the pressure or the normal component of the flux must be defined. There must be at least one point where the pressure is prescribed. The method will try to cast the given values to appropriate `Data` class objects.

getSolverOptionsFlux()

returns the solver options used to solve the flux problems. Use this `SolverOptions` object to control the solution algorithms. This option is only relevant if global postprocesing is used.

getSolverOptionsPressure()

returns a `SolverOptions` object with the options used to solve the pressure problems. Use this object to control the solution algorithms.

solve(u0,p0)

solves the problem and returns approximations for the flux v and the pressure p. `u0` and `p0` define initial guesses for flux and pressure. Values marked by positive values `location_of_fixed_flux` and `location_of_fixed_pressure`, respectively, are kept unchanged.

getFlux(p, [u0 = None])

returns the flux for a given pressure `p` where the flux is equal to `u0` on locations where `location_of_fixed_flux` is positive, see `setValue`. Notice that `g` and `f` are used.

6.3 Isotropic Kelvin Material

As proposed by Kelvin [20] material strain $D_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i})$ can be decomposed into an elastic part D^{el}_{ij} and a visco-plastic part D^{vp}_{ij}:

$$D_{ij} = D^{el}_{ij} + D^{vp}_{ij} \tag{6.42}$$

with the elastic strain given as

$$D^{el'}_{ij} = \frac{1}{2\mu}\dot{\sigma}'_{ij} \tag{6.43}$$

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

$$D^{vp'}_{ij} = \sum_q D^{q'}_{ij} \tag{6.44}$$

where D^q_{ij} is the strain in material q given as

$$D^{q'}_{ij} = \frac{1}{2\eta^q}\sigma'_{ij} \tag{6.45}$$

and η^q is the viscosity of material q. We assume the following between the strain in material q

$$\eta^q = \eta^q_N \left(\frac{\tau}{\tau^q_t}\right)^{1-n^q} \quad \text{with } \tau = \sqrt{\frac{1}{2}\sigma'_{ij}\sigma'_{ij}} \tag{6.46}$$

for given power law coefficients $n^q \geq 1$ and transition stresses τ_t^q, see [20]. Notice that $n^q = 1$ gives a constant viscosity. After inserting Equation (6.45) into Equation (6.44) one gets:

$$D_{ij}^{\prime vp} = \frac{1}{2\eta^{vp}}\sigma_{ij}^{\prime} \text{ with } \frac{1}{\eta^{vp}} = \sum_q \frac{1}{\eta^q} \ . \tag{6.47}$$

and finally with 6.42

$$D_{ij}^{\prime} = \frac{1}{2\eta^{vp}}\sigma_{ij}^{\prime} + \frac{1}{2\mu}\dot{\sigma}_{ij}^{\prime} \tag{6.48}$$

The total stress τ needs to fulfill the yield condition

$$\tau \leq \tau_Y + \beta\, p \tag{6.49}$$

with the Drucker-Prager cohesion factor τ_Y, Drucker-Prager friction β and total pressure p. The deviatoric stress needs to fulfill the equilibrium equation

$$-\sigma_{ij,j}^{\prime} + p_{,i} = F_i \tag{6.50}$$

where F_j is a given external force. We assume an incompressible medium:

$$-v_{i,i} = 0 \tag{6.51}$$

Natural boundary conditions are taken in the form

$$\sigma_{ij}^{\prime} n_j - n_i p = f \tag{6.52}$$

which can be overwritten by a constraint

$$v_i(x) = 0 \tag{6.53}$$

where the index i may depend on the location x on the boundary.

6.3.1 Solution Method

By using a first order finite difference approximation with step size $dt > 0$ Equation (6.43) is transformed to

$$\dot{\sigma}_{ij} = \frac{1}{dt}\left(\sigma_{ij} - \sigma_{ij}^{-}\right) \tag{6.54}$$

and

$$D_{ij}^{\prime} = \left(\frac{1}{2\eta^{vp}} + \frac{1}{2\mu dt}\right)\sigma_{ij}^{\prime} - \frac{1}{2\mu dt}\sigma_{ij}^{-\prime} \tag{6.55}$$

where σ_{ij}^{-} is the stress at the previous time step. With

$$\dot{\gamma} = \sqrt{2\left(D_{ij}^{\prime} + \frac{1}{2\mu\ dt}\sigma_{ij}^{-\prime}\right)^2} \tag{6.56}$$

we have

$$\tau = \eta_{eff} \cdot \dot{\gamma} \tag{6.57}$$

where

$$\eta_{eff} = min(\left(\frac{1}{\mu\ dt} + \frac{1}{\eta^{vp}}\right)^{-1}, \eta_{max}) \text{ with } \eta_{max} = \begin{cases} \frac{\tau_Y + \beta\ p}{\dot{\gamma}} & \dot{\gamma} > 0 \\ \text{if} & \\ \infty & \text{otherwise} \end{cases} \tag{6.58}$$

The upper bound η_{max} makes sure that yield condition 6.49 holds. With this setting the equation 6.55 takes the form

$$\sigma_{ij}^{\prime} = 2\eta_{eff}\left(D_{ij}^{\prime} + \frac{1}{2\mu\ dt}\sigma_{ij}^{\prime -}\right) \tag{6.59}$$

After inserting 6.59 into 6.50 we get

$$-\left(\eta_{eff}(v_{i,j} + v_{i,j})\right)_{,j} + p_{,i} = F_i + \left(\frac{\eta_{eff}}{\mu dt}\sigma_{ij}^{\prime -}\right)_{,j} \tag{6.60}$$

Combining this with the incompressibility condition 6.42 we need to solve a Stokes problem as discussed in Section 6.1.1 in each time step.

If we set

$$\frac{1}{\eta(\tau)} = \frac{1}{\mu\ dt} + \frac{1}{\eta^{vp}} \tag{6.61}$$

we need to solve the nonlinear problem

$$\eta_{eff} - min(\eta(\dot{\gamma} \cdot \eta_{eff}), \eta_{max}) = 0 \tag{6.62}$$

We use the Newton-Raphson scheme to solve this problem:

$$\eta_{eff}^{(n+1)} = \min(\eta_{max}, \eta_{eff}^{(n)} - \frac{\eta_{eff}^{(n)} - \eta(\tau^{(n)})}{1 - \dot{\gamma} \cdot \eta'(\tau^{(n)})}) = \min(\eta_{max}, \frac{\eta(\tau^{(n)}) - \tau^{(n)} \cdot \eta'(\tau^{(n)})}{1 - \dot{\gamma} \cdot \eta'(\tau^{(n)})}) \tag{6.63}$$

where η' denotes the derivative of η with respect to τ and $\tau^{(n)} = \dot{\gamma} \cdot \eta_{eff}^{(n)}$. Looking at the evaluation of η in 6.61 it makes sense to formulate the iteration 6.63 using $\Theta = \eta^{-1}$. In fact we have

$$\eta' = -\frac{\Theta'}{\Theta^2} \text{ with } \Theta' = \sum_q \left(\frac{1}{\eta^q}\right)' \tag{6.64}$$

As

$$\left(\frac{1}{\eta^q}\right)' = \frac{n^q - 1}{\eta_N^q} \cdot \frac{\tau^{n^q-2}}{(\tau_t^q)^{n^q-1}} = \frac{n^q - 1}{\eta^q} \cdot \frac{1}{\tau} \tag{6.65}$$

we have

$$\Theta' = \frac{1}{\tau}\omega \text{ with } \omega = \sum_q \frac{n^q - 1}{\eta^q} \tag{6.66}$$

which leads to

$$\eta_{eff}^{(n+1)} = \min(\eta_{max}, \eta_{eff}^{(n)} \frac{\Theta^{(n)} + \omega^{(n)}}{\eta_{eff}^{(n)}\Theta^{(n)^2} + \omega^{(n)}}) \tag{6.67}$$

6.3.2 Functions

class IncompressibleIsotropicFlowCartesian(domain [, stress=0 [, v=0 [, p=0 [, t=0 [, numMaterials=1 [, verbose=True [, adaptSubTolerance=True]]]]]]])

opens an incompressible, isotropic flow problem in Cartesian coordinates on the domain `domain`. `stress`, `v`, `p`, and `t` set the initial deviatoric stress, velocity, pressure and time. `numMaterials` specifies the number of materials used in the power law model. Some progress information is printed if `verbose` is set to *True*. If `adaptSubTolerance` is equal to *True* the tolerances for subproblems are set automatically.

The domain needs to support LBB compliant elements for the Stokes problem, see [12] for details. For instance one can use second order polynomials for velocity and first order polynomials for the pressure on the same element. Alternatively, one can use macro elements using linear polynomials for both pressure and velocity but with a subdivided element for the velocity. Typically, the macro element method is more cost effective. The fact that pressure and velocity are represented in different ways is expressed by

```
velocity=Vector(0.0, Solution(mesh))
pressure=Scalar(0.0, ReducedSolution(mesh))
```

getDomain()

returns the domain.

getTime()

returns current time.

getStress()

returns current stress.

getDeviatoricStress()
returns current deviatoric stress.

getPressure()
returns current pressure.

getVelocity()
returns current velocity.

getDeviatoricStrain()
returns deviatoric strain of current velocity

getTau()
returns current second invariant of deviatoric stress

getGammaDot()
returns current second invariant of deviatoric strain

setTolerance(tol=1.e-4)
sets the tolerance used to terminate the iteration on a time step.

setFlowTolerance(tol=1.e-4)
sets the relative tolerance for the incompressible solver, see `StokesProblemCartesian` for details.

setElasticShearModulus(mu=None)
sets the elastic shear modulus μ. If `mu` is set to None (default) elasticity is not applied.

setEtaTolerance=(rtol=1.e-8)
sets the relative tolerance for the effective viscosity. Iteration on a time step is completed if the relative of the effective viscosity is less than `rtol`.

setDruckerPragerLaw([tau_Y=None, [friction=None]])
sets the parameters τ_Y and β for the Drucker-Prager model in condition 6.49. If `tau_Y` is set to None (default) then the Drucker-Prager condition is not applied.

setElasticShearModulus(mu=None)
sets the elastic shear modulus μ. If `mu` is set to None (default) elasticity is not applied.

setPowerLaws(eta_N, tau_t, power)
sets the parameters of the power-law for all materials as defined in Equation (6.46). `eta_N` is the list of viscosities η_N^q, `tau_t` is the list of reference stresses τ_t^q, and `power` is the list of power law coefficients n^q.

update(dt [, iter_max=100 [, inner_iter_max=20]])
updates stress, velocity and pressure for time increment `dt`, where `iter_max` is the maximum number of iteration steps on a time step to update the effective viscosity and `inner_iter_max` is the maximum number of iteration steps in the incompressible solver.

6.4 Fault System

The `FaultSystem` class provides an easy-to-use interface to handle 2D and 3D fault systems as used for instance in simulating fault ruptures. The main purpose of the class is to provide a parameterization of an individual fault

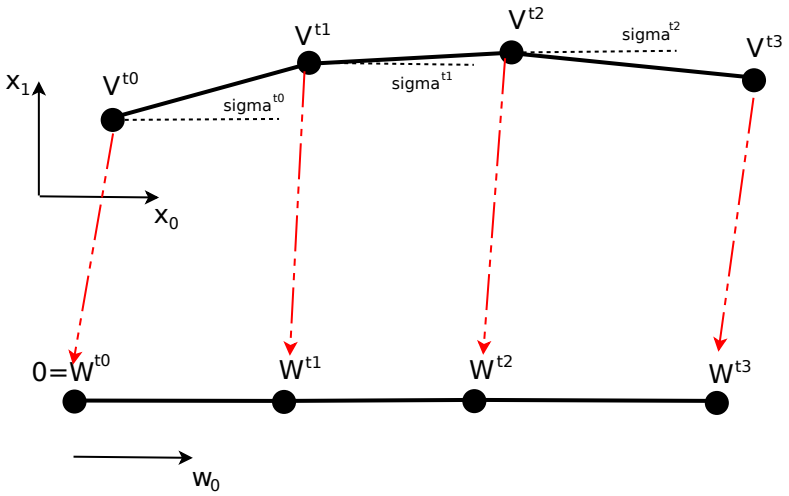


FIGURE 6.1: Two dimensional fault system with one fault named 't' in the (x_0, x_1) space and its parameterization in the w_0 space. The fault has three segments.

in the system of faults. In case of a 2D fault the fault is parameterized by a single value w_0 and in the case of a 3D fault two parameters w_0 and w_1 are used. This parameterization can be used to impose data (e.g. a slip distribution) onto the fault. It can also be a useful tool to visualize or analyze the results on the fault if the fault is not straight.

A fault t in the fault system is represented by a starting point V^{t0} and series of directions, called strikes, and the lengths (l^{ti}). The strike of segment i is defined by the angle σ^{ti} between the x_0-axis and the direction of the fault, see Figure 6.1. The length and strike defines the polyline (V^{ti}) of the fault by

$$V^{ti} = V^{t(i-1)} + l^{ti} \cdot S^{ti} \text{ with } S^{ti} = \begin{bmatrix} cos(\sigma^{ti}) \\ sin(\sigma^{ti}) \\ 0 \end{bmatrix} \tag{6.68}$$

In the 3D case each fault segment i has an additional dip θ^{ti} and at each vertex i a depth δ^{ti} is given. The fault segment normal n^{ti} is given by

$$n^{ti} = \begin{bmatrix} -sin(\theta^{ti}) \cdot S_1^{ti} \\ sin(\theta^{ti}) \cdot S_0^{ti} \\ cos(\theta^{ti}) \end{bmatrix} \tag{6.69}$$

At each vertex we define a depth vector d^{ti} defined as the intersect of the fault planes of segment $(i-1)$ and i where for the first segment and last segment the vector orthogonal to strike vector S^{ti} and the segment normal n^{ti} is used. The direction $\tilde{d}^{ti}$ of the depth vector is given as

$$\tilde{d}^{ti} = n^{ti} \times n^{t(i-1)} \tag{6.70}$$

If $\tilde{d}^{ti}$ is zero the strike vectors $L^{t(i-1)}$ and L^{ti} are collinear and we can set $\tilde{d}^{ti} = l^{ti} \times n^{ti}$. If the two fault segments are almost orthogonal $\tilde{d}^{ti}$ is pointing in the direction of $L^{t(i-1)}$ and L^{ti}. In this case no depth can be defined. So we will reject a fault system if

$$min(\|\tilde{d}^{ti} \times L^{t(i-1)}\|, \|\tilde{d}^{ti} \times L^{ti}\|) \leq 0.1 \cdot \|\tilde{d}^{ti}|\tag{6.71}$$

which corresponds to an angle of less than 10^o between the depth vector and the strike. We then set

$$d^{ti} = \delta^{ti} \cdot \frac{\tilde{d}^{ti}}{\|\tilde{d}^{ti}\|} \tag{6.72}$$

We can then define the polyline (v^{ti}) for the bottom of the fault as

$$v^{ti} = V^{ti} + d^{ti} \tag{6.73}$$

In order to simplify working on a fault t in a fault system a parameterization $P^t : (w_0, w_1) \to (x_0, x_1, x_2)$ over a rectangular domain is introduced such that

$$0 \leq w_0 \leq w^t_{0max} \text{ and } -w^t_{1max} \leq w_1 \leq 0 \tag{6.74}$$

with positive numbers w^t_{0max} and w^t_{1max}. Typically one chooses w^t_{0max} to be the unrolled length of the fault and w^t_{1max} to be the mean value of segment depth. Moreover we have

$$P^t(W^{ti}) = V^{ti} \text{ and } P^t(w^{ti}) = v^{ti} \tag{6.75}$$

where

$$W^{ti} = (\Omega^{ti}, 0) \text{ and } w^{ti} = (\Omega^{ti}, -w^t_{1max}) \tag{6.76}$$

and Ω^{ti} is the unrolled distance of W^{ti} from W^{t0}, i.e. $l^{ti} = \Omega^{t(i+1)} - \Omega^{ti}$. In the 2D case w^t_{1max} is set to zero and therefore the second component is dropped, see Figure 6.1.

In the 2D case the parameterization P^t is constructed as follows: The line connecting $V^{t(i-1)}$ and V^{ti} is given by

$$x = V^{ti} + s \cdot (V^{t(i+1)} - V^{ti}) \tag{6.77}$$

where s is between 0 and 1. The point x is on i-th fault segment if and only if such an s exists. Assuming x is on the fault it can be calculated as

$$s = \frac{(x - V^{ti})^t \cdot (V^{t(i+1)} - V^{ti})}{\|V^{t(i+1)} - V^{ti}\|^2} \tag{6.78}$$

We then can set

$$w_0 = \Omega^{ti} + s \cdot (\Omega^{ti} - \Omega^{t(i-1)}) \tag{6.79}$$

to get $P^t(w_0) = x$. It remains the question if the given x is actually on the segment i of fault t. To test this s is restricted between 0 and 1 (so if $s < 0$, s is set to 0 and if $s > 1$, s is set to 1) and then we check the residual of Equation (6.77), i.e. x has been accepted to be in the segment if

$$\|x - V^{ti} - s \cdot (V^{t(i+1)} - V^{ti})\| \leq tol \cdot max(l^{ti}, \|x - V^{ti}\|) \tag{6.80}$$

where tol is a given tolerance.

In the 3D case the situation is a bit more complicated: we split the fault segment across the diagonal V^{ti}-$v^{t(i+1)}$ to produce two triangles. In the upper triangle we use the parameterization

$$x = V^{ti} + s \cdot (V^{t(i+1)} - V^{ti}) + r \cdot (v^{t(i+1)} - V^{t(i+1)}) \text{ with } r \leq s; \tag{6.81}$$

while in the lower triangle we use

$$x = V^{ti} + s \cdot (v^{t(i+1)} - v^{ti}) + r \cdot (v^{ti} - V^{ti}) \text{ with } s \leq r; \tag{6.82}$$

where $0 \leq s, r \leq 1$. Both equations are solved in the least-squares sense e.g. using the MoorePenrose pseudo-inverse for the coefficient matrices. The resulting s and r are then restricted to the unit square. Similar to the 2D case (see Equation (6.80)) we identify x to be in the upper triangle of the segment if

$$\|x - V^{ti} - s \cdot (V^{t(i+1)} - V^{ti}) - r \cdot (v^{t(i+1)} - V^{t(i+1)})\| \leq tol \cdot max(\|x - V^{ti}\|, \|v^{t(i+1)} - V^{t(i)})\|) \tag{6.83}$$

and in the lower part

$$\|x - V^{ti} - s \cdot (v^{t(i+1)} - v^{ti}) - r \cdot (v^{ti} - V^{ti})\| \leq tol \cdot max(\|x - V^{ti}\|, \|v^{t(i+1)} - V^{t(i)})\|) \tag{6.84}$$

after the restriction of (s, t) to the unit square. Note that $\|v^{t(i+1)} - V^{t(i)})\|$ is the length of the diagonal of the fault segment. For those x which have been located in the i-th segment we then set

$$w_0 = \Omega^{ti} + s \cdot (\Omega^{ti} - \Omega^{t(i-1)}) \text{ and } w_1 = w^t_{1max}(r - 1) \tag{6.85}$$

6.4.1 Functions

class FaultSystem([dim =3])
creates a fault system in the `dim` dimensional space.

getMediumDepth(tag)
returns the medium depth of fault `tag`.

getTags()
returns a list of the tags used by the fault system.

getStart(tag)
returns the starting point of fault `tag` as a `numpy.ndarray` object.

getDim()
returns the spatial dimension.

getDepths(tag)
returns the list of the depths of the segments in fault `tag`.

getTopPolyline(tag)
returns the polyline used to describe the fault tagged by `tag`.

getStrikes(tag)
returns the list of strikes σ^{ti} of the segments in fault $t =$`tag`.

getStrikeVectors(tag)
returns the strike vectors S^{ti} of fault $t =$`tag`.

getLengths(tag)
returns the lengths l^{ti} of the segments in fault $t =$`tag`.

getTotalLength(tag)
returns the total unrolled length of fault `tag`.

getDips(tag)
returns the list of the dips of the segments in fault `tag`.

getBottomPolyline(tag)
returns the list of the vertices defining the bottom of the fault `tag`.

getSegmentNormals(tag)
returns the list of the normals of the segments in fault `tag`.

getDepthVectors(tag)
returns the list of the depth vectors d^{ti} for fault $t =$`tag`.

getDepths(tag)
returns the list of the depths of the segments in fault `tag`.

getW0Range(tag)
returns the range of the parameterization in w_0. For tag t this is the pair $(\Omega^{t0}, \Omega^{tn})$ where n is the number of segments in the fault. In most cases one has $(\Omega^{t0}, \Omega^{tn}) = (0, w^t_{0max})$.

getW1Range(tag)
returns the range of the parameterization in w_1. For tag t this is the pair $(-w^t_{1max}, 0)$.

getW0Offsets(tag)
returns the offsets for the parameterization of fault `tag`. For tag `tag` =t this is the list $[\Omega^{ti}]$.

getCenterOnSurface()
returns the center point of the fault system at the surfaces. In 3D the calculation of the center is considering the top edge of the faults and projects the edge to the surface (the x_2 component is assumed to be 0). An `numpy.ndarray` object is returned.

getOrientationOnSurface()
returns the orientation of the fault system in RAD on the surface ($x_2 = 0$ plane) around the fault system center.

transform([rot=0, [shift=numpy.zeros((3,)]])
applies a shift `shift` and a consecutive rotation in the $x_2 = 0$ plane. `rot` is a float number and `shift` an `numpy.ndarray` object.

getMaxValue(f[, tol=1.e-8])
returns the tag of the fault where `f` takes the maximum value and a `Locator` object which can be used to collect values from `Data` objects at the location where the maximum is taken, e.g.

```
fs=FaultSystem()
f=Scalar(..)
t, loc=fs.getMaxValue(f)
print("maximum value of f on the fault %s is %s at location %s."%(t, \
      loc(f), loc.getX()))
```

`f` must be a scalar `Data` object. When the maximum is calculated only data sample points are considered which are on a fault in the fault system in the sense of condition 6.80 or 6.84, respectively. In the case no data sample points are found the returned tag is `None` and the maximum value as well as the location of the maximum value are undefined.

getMinValue(f[, tol=1.e-8])
returns the tag of the fault where `f` takes the minimum value and a `Locator` object which can be used to collect values from `Data` objects at the location where the minimum is taken, e.g.

```
fs=FaultSystem()
f=Scalar(..)
t, loc=fs.getMinValue(f)
print "minimum value of f on the fault %s is %s at location."%(t,loc(f),loc.getX())
```

`f` must be a scalar `Data` object. When the minimum is calculated only data sample points are considered which are on a fault in the fault system in the sense of condition 6.80 or 6.84, respectively. In the case no data sample points are found the returned tag is `None` and the minimum value as well as the location of the minimum value are undefined.

getParametrization(x,tag [[, tol=1.e-8], outsider=None])
returns the argument w of the parameterization P^t for `tag` =t to provide `x` together with a mask indicating where the given location if on a fault in the fault system by the value 1 (otherwise the value is set to 0). `x` needs to be a vector `Data` object or `numpy.ndarray` object. `tol` defines the tolerance to decide if given data sample points are on fault `tag`. The value `outside` is the value used as a replacement value for w where the corresponding value in `x` is not on a fault. If `outside` is not present an appropriate value is used.

getSideAndDistance(x,tag)

returns the side and the distance at locations `x` from the fault `tag`. `x` needs to be a vector `Data` object or `numpy.ndarray` object. Positive values for side means that the corresponding location is to the right of the fault, a negative value means that the corresponding location is to the left of the fault. The value zero means that the side is undefined.

getFaultSegments(tag)

returns the polylines used to describe fault `tag`. For `tag` =t this is the list of the vertices $[V^{ti}]$ for the 2D and the pair of lists of the top vertices $[V^{ti}]$ and the bottom vertices $[v^{ti}]$ in 3D. Note that the coordinates are represented as `numpy.ndarray` objects.

addFault(strikes[, ls[, V0=[0.,0.,0.][, tag=None[, dips=None[, depths= None[, w0_offsets=None[, w1_max=None]]]]]]])

adds the fault `tag` to the fault system. `V0` defines the start point of fault named t =`tag`. The polyline defining the fault segments on the surface are set by the strike angles `strikes` (=σ^{ti}, north = $\pi/2$, the orientation is counterclockwise.) and the length `ls` (=l^{ti}). In the 3D case one also needs to define the dip angles `dips` (=δ^{ti}, vertical=0, right-hand rule applies.) and the depth `depths` for each segment. `w1_max` defines the range of w_1. If not present the mean value over the depth of all segment edges in the fault is used. `w0_offsets` sets the offsets Ω^{ti}. If not present it is chosen such that $\Omega^{ti} - \Omega^{t(i-1)}$ is the length of the i-th segment. In some cases, e.g. when kinks in the fault are relevant, it can be useful to explicitly specify the offsets in order to simplify the assignment of values.

6.4.2 Example

See Section 1.6.

CHAPTER
SEVEN

The `esys.finley` Module

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 access to the library through the `LinearPDE` class of `esys.escript` supporting its full functionality. *finley* is parallelized using the OpenMP paradigm.

7.1 Formulation

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

$$\begin{aligned} & \int_\Omega A_{jl} \cdot v_{,j} u_{,l} + B_j \cdot v_{,j} u + C_l \cdot v u_{,l} + D \cdot v u \, d\Omega \\ + & \int_\Gamma d \cdot v u \, d\Gamma + \int_{\Gamma^{contact}} d^{contact} \cdot [v][u] \, d\Gamma \\ = & \int_\Omega X_j \cdot v_{,j} + Y \cdot v \, d\Omega \\ + & \int_\Gamma y \cdot v \, d\Gamma + \int_{\Gamma^{contact}} y^{contact} \cdot [v] \, d\Gamma \end{aligned} \tag{7.1}$$

7.2 Meshes

To understand the usage of `esys.finley` one needs to have an understanding of how the finite element meshes are defined. Figure 7.1 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. quadrilaterals or, in the three-dimensional case, into tetrahedra and hexahedra. 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 its boundary to neighbour elements. In the example of Figure 7.1 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 parameterization 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 [38, 4] for more details. `esys.finley` also supports macro elements. For these elements a piecewise linear approximation is used on an element which is further subdivided (in the case of `esys.finley` halved). As such, these elements do not provide more than a further mesh refinement but should be used in the case of incompressible flows, see `StokesProblemCartesian`. For these problems a linear approximation of the pressure across the element is used (use the reduced solution `FunctionSpace`) while the refined element is used to approximate velocity. So a macro element provides a continuous pressure approximation together with a velocity approximation on a refined mesh. This approach is necessary to make sure that the incompressible flow has a unique solution.

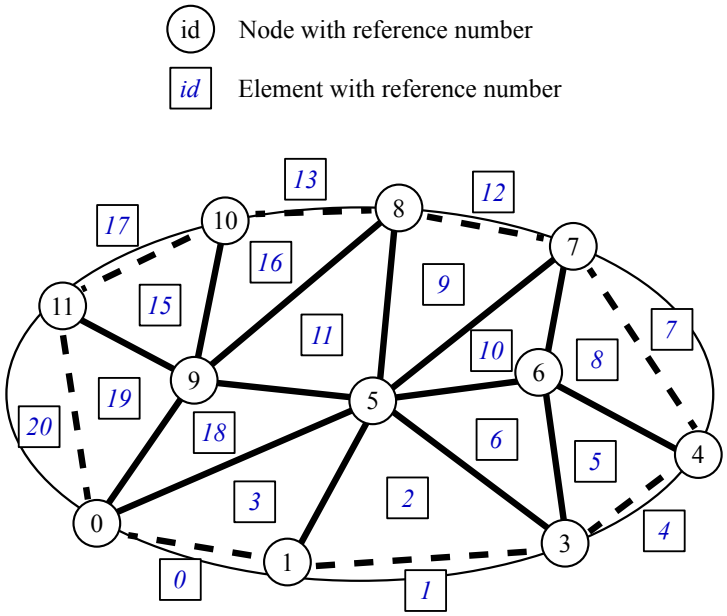


FIGURE 7.1: Subdivision of an Ellipse into triangles order 1 (*Tri3*)

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 7.1 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 7.1 line elements with two nodes are used. The elements are also defined by their describing nodes, e.g. the face element with 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-dimensional 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 need to be used. Rich elements on a face are identical to interior elements but with a modified order of nodes such that the 'first' face of the element aligns with the surface of the domain. In Figure 7.1 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 7.2 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 and 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 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 7.1 shows the interior element types and the corresponding element types to be used on the face and contacts. Figure 7.3, Figure 7.4 and Figure 7.5 show the ordering of the nodes within an element.

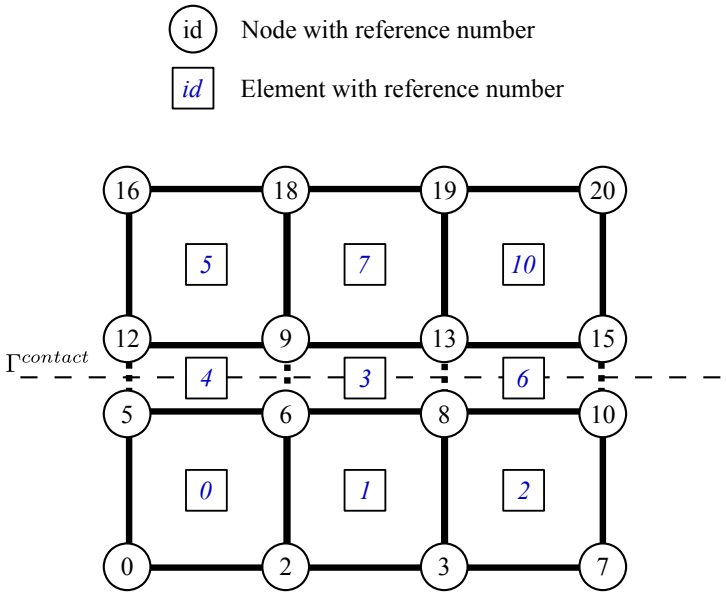


FIGURE 7.2: Mesh around a contact region (*Rec4*)

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 a 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 of these is crucial. Each element 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 tag 2 and elements below a contact region are marked with tag 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")
```

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*
Hex27	*Rec9*	N/A	N/A	N/A
Hex27Macro	*Rec9Macro*	N/A	N/A	N/A
Tet10Macro	*Tri6Macro*	N/A	N/A	N/A
Rec9Macro	*Line3Macro*	N/A	N/A	N/A
Tri6Macro	*Line3Macro*	N/A	N/A	N/A

Table 7.1: Finley elements and corresponding elements to be used on domain faces and contacts. The rich types have to be used if the gradient of the function is to be calculated on faces and contacts, respectively.

```
# point sources (not supported yet)
print("Point1 0")
```

The following example of a mesh file defines the mesh shown in Figure 7.2:

```
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 conditions 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 $x_0 = 0$ and $x_0 = 1$ 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 now reads:

```
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
```

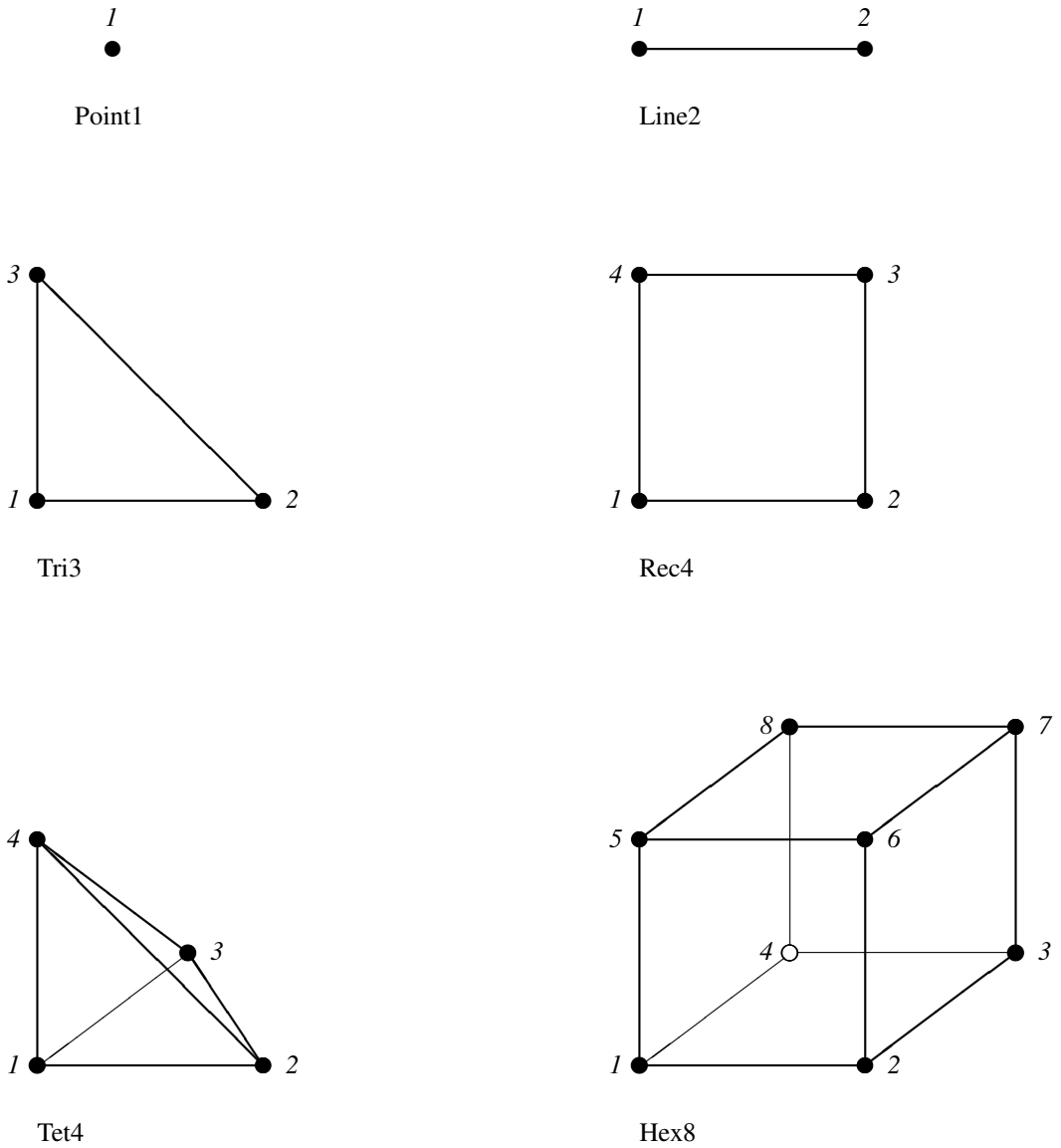


FIGURE 7.3: Elements of order 1

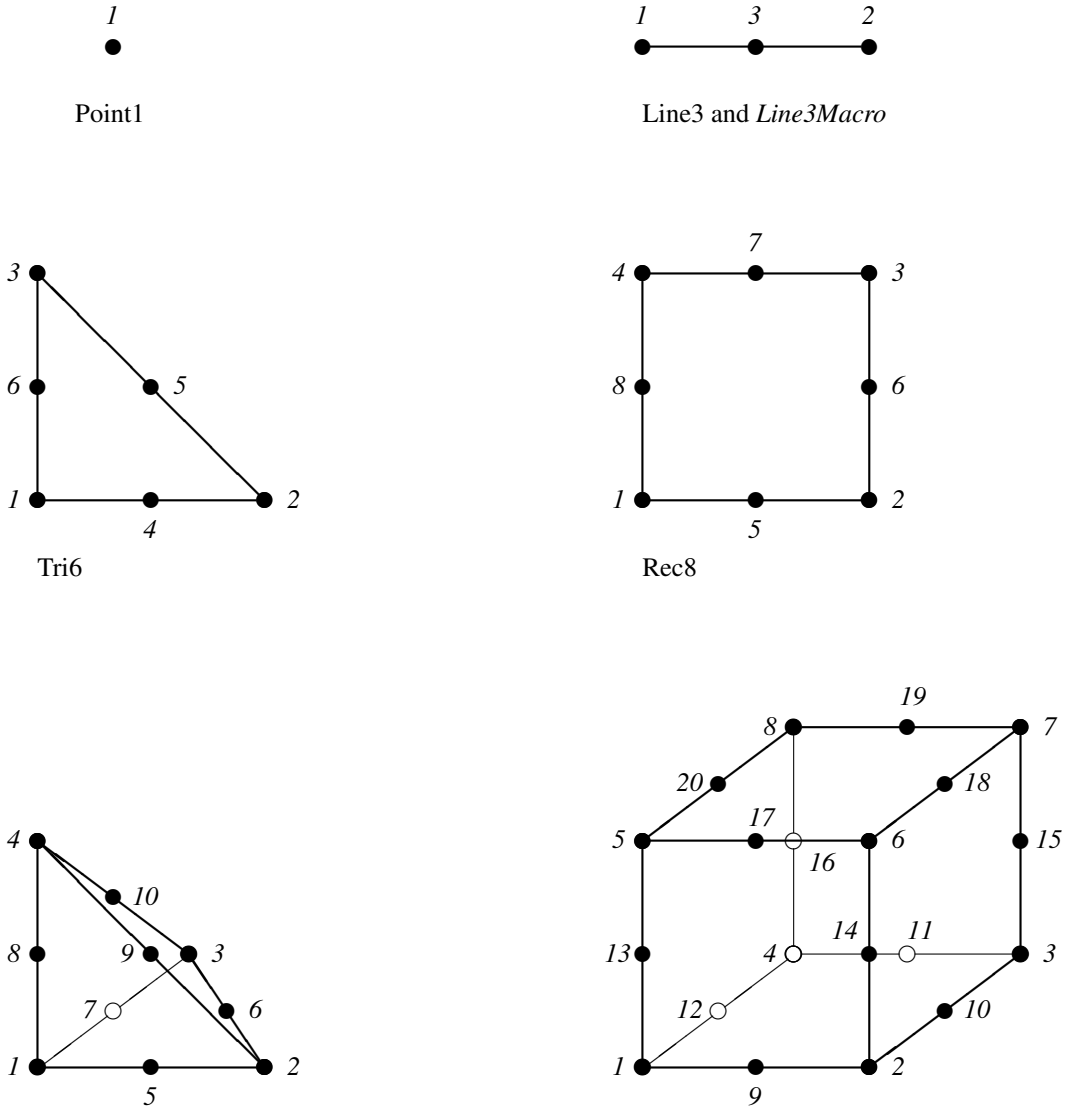


FIGURE 7.4: Elements of order 2 and macro elements

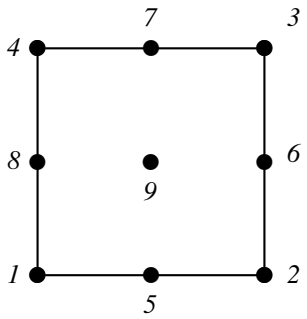
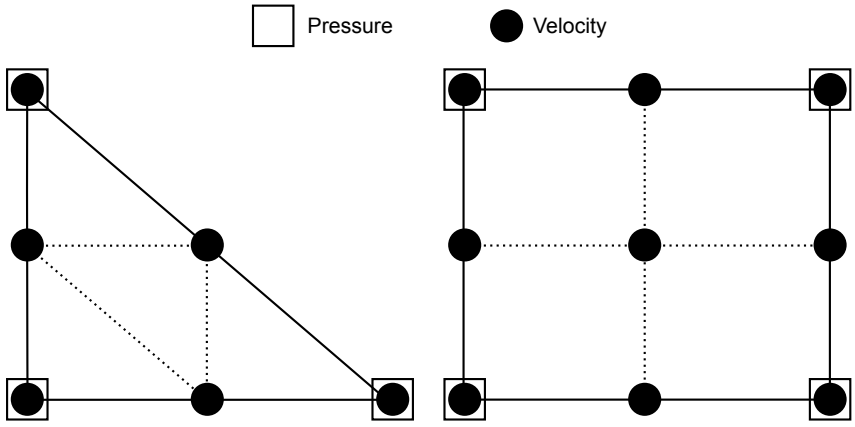


FIGURE 7.5: *Rec9* and *Rec9Macro*

7.3 Macro Elements



(a) Triangle (b) Quadrilateral

FIGURE 7.6: Macro elements in `esys.finley`

`esys.finley` supports the usage of macro elements which can be used to achieve LBB compliance when solving incompressible fluid flow problems. LBB compliance is required to get a problem which has a unique solution for pressure and velocity. For macro elements the pressure and velocity are approximated by a polynomial of order 1 but the velocity approximation bases on a refinement of the elements. The nodes of a triangle and quadrilateral element are shown in Figures 7.6(a) and 7.6(b), respectively. In essence, the velocity uses the same nodes like a quadratic polynomial approximation but replaces the quadratic polynomial by piecewise linear polynomials. In fact, this is the way `esys.finley` defines the macro elements. In particular `esys.finley` uses the same local ordering of the nodes for the macro element as for the corresponding quadratic element. Another interpretation is that one uses a linear approximation of the velocity together with a linear approximation of the pressure but on elements created by combining elements to macro elements. Notice that the macro elements still use quadratic interpolation to represent the element and domain boundary. However, if elements have linear boundaries a macro element approximation for the velocity is equivalent to using a linear approximation on a mesh which is created through a one-step global refinement. Typically macro elements are only required to use when an incompressible fluid flow problem is solved, e.g. the Stokes problem in Section 6.1. Please see Section 7.2 for more details on the supported macro elements.

7.4 Linear Solvers in `SolverOptions`

Table 7.2 and Table 7.3 show the solvers and preconditioners supported by `esys.finley` through the `PASO` library. Currently direct solvers are not supported under *MPI*. By default, `esys.finley` uses the iterative solvers `SolverOptions.PCG` for symmetric and `SolverOptions.BICGSTAB` for non-symmetric problems. If the direct solver is selected, which can be useful when solving very ill-posed equations, `esys.finley` uses the `MKL` [1] solver package. If `MKL` is not available `UMFPACK` is used. If `UMFPACK` is not available a suitable iterative solver from `PASO` is used.

7.5 Functions

ReadMesh(fileName [, [integrationOrder=-1], optimize=True])

creates a `Domain` object from the FEM mesh defined in file `fileName`. The file must be in the `esys.finley` file format. If `integrationOrder` is positive, a numerical integration scheme is chosen which is accurate on each element up to a polynomial of degree `integrationOrder` . Otherwise an

[1] If the stiffness matrix is non-regular `MKL` may return without a proper error code. If you observe suspicious solutions when using `MKL` , this may be caused by a non-invertible operator.

setSolverMethod	DIRECT	PCG	GMRES	TFQMR	MINRES	PRES20	BICGSTAB	lumping
setReordering	✓							
setRestart			✓			20		
setTruncation			✓			5		
setIterMax		✓	✓	✓	✓	✓	✓	
setTolerance		✓	✓	✓	✓	✓	✓	
setAbsoluteTolerance		✓	✓	✓	✓	✓	✓	
setReordering	✓							

Table 7.2: Solvers available for esys.finley and the PASO package and the relevant options in SolverOptions. MKL supports MINIMUM_FILL_IN and NESTED_DISSECTION reordering. Currently the UMFPACK interface does not support any reordering.

NO_PRECONDITIONER	AMG	JACOBI	GAUSS_SEIDEL	REC_ILU	RILU	ILU0	DIRECT
status:	✓	✓	✓	✓	later	✓	later
setLevelMax	✓						
setCoarseningThreshold	✓						
setMinCoarseMatrixSize	✓						
setMinCoarseMatrixSparsity	✓						
setNumSweeps		✓	✓				
setNumPreSweeps	✓						
setNumPostSweeps	✓						
setDiagonalDominanceThreshold	✓						
setAMGInterpolation	✓						
setRelaxationFactor					✓		

Table 7.3: Preconditioners available for esys.finley and the PASO package and the relevant options in SolverOptions.

appropriate integration order is chosen independently. By default the labeling of mesh nodes and element distribution is optimized. Set optimize=False to switch off relabeling and redistribution.

ReadGmsh(fileName [, [integrationOrder=-1], optimize=True[, useMacroElements=False]])
creates a Domain object from the FEM mesh defined in file fileName. The file must be in the *Gmsh*[11] file format. If integrationOrder is positive, a numerical integration scheme is chosen which is accurate on each element up to a polynomial of degree integrationOrder . Otherwise an appropriate integration order is chosen independently. By default the labeling of mesh nodes and element distribution is optimized. Set optimize=False to switch off relabeling and redistribution. If useMacroElements is set, second order elements are interpreted as macro elements. Currently ReadGmsh does not support *MPI*.

MakeDomain(design[, integrationOrder=-1[, optimizeLabeling=True[, useMacroElements=False]]])
creates a esys.finley Domain from a esys.pycad Design object using *Gmsh*[11]. The Design design defines the geometry. If integrationOrder is positive, a numerical integration scheme is chosen which is accurate on each element up to a polynomial of degree integrationOrder . Otherwise an appropriate integration order is chosen independently. Set optimizeLabeling=False to switch off relabeling and redistribution (not recommended). If useMacroElements is set, macro elements are used. Currently MakeDomain does not support *MPI*.

load(fileName)
recovers a Domain object from a dump file fileName created by the dump method of a Domain object.

Rectangle(n0,n1,order=1,l0=1.,l1=1., integrationOrder=-1,
periodic0=*False*, periodic1=*False*, useElementsOnFace=*False*, useMacroElements=*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 x_0-axis and n1 elements along the x_1-axis. For order =1 and order =2, elements of type *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. If order =-1, *Rec8Macro* and *Line3Macro* are used. This option should be used when solving incompressible fluid flow problems, e.g. StokesProblemCartesian. 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 is 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 x_0-direction are enforced. That means for any solution of a PDE solved by `esys.finley` the values on the line $x_0 = 0$ will be identical to the values on $x_0 =$ `l0`. Correspondingly, `periodic1` =*True* sets periodic boundary conditions in the x_1-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*, useMacroElements=*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 x_0-axis, `n1` elements along the x_1-axis and `n2` elements along the x_2-axis. For `order` =1 and `order` =2, elements of type *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 `order` =-1, *Hex20Macro* and *Rec8Macro* are used. This option should be used when solving incompressible fluid flow problems, e.g. `StokesProblemCartesian`. If `integrationOrder` is positive, a numerical integration scheme is 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 x_0-direction are enforced. That means for any solution of a PDE solved by `esys.finley` the values on the plane $x_0 = 0$ will be identical to the values on $x_0 =$ `l0`. Correspondingly, `periodic1` =*True* and `periodic2` =*True* sets periodic boundary conditions in the x_1-direction and x_2-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, 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 than `tolerance` times the diameter of the domain are merged. The corresponding face elements are removed from the mesh. `GlueFaces` is not supported under *MPI* with more than one rank.

JoinFaces(meshList, tolerance=1.e-13)

generates a new `Domain` object from the list `meshList` of `esys.finley` meshes. Face elements whose node coordinates differ by less than `tolerance` times the diameter of the domain are combined to form a contact element. The corresponding face elements are removed from the mesh. `JoinFaces` is not supported under *MPI* with more than one rank.

CHAPTER
EIGHT

The `esys.weipa` Module and Data Visualization

The *weipa* C++ library and accompanying *python* module allow exporting `esys.escript Data` objects and their domain in a format suitable for visualization. Besides creating output files, *weipa* can also interface with the *VisIt* visualization software. This allows accessing the latest simulation data while the simulation is still running without the need to save any files.

8.1 The `EscriptDataset` class

class EscriptDataset()
holds an *escript* dataset including a domain and data variables for a single time step and offers methods to export the data in various formats. It is preferable to create a dataset object using the `createDataset` function from `esys.weipa` (see Section 8.2) rather than using the (non-exposed) *python* constructor for the class.

The following methods are available:

setDomain(domain)
sets the `Domain` for this dataset. Note that the domain can only be set once and all `Data` objects added to this dataset must be defined on the same domain.

addData(data, name [, units=""])
adds the `Data` object `data` to this dataset which will be exported by the given `name`. Some export formats support data units which can be set through the `units` parameter, e.g. `"km/h"`. Before calling this method a domain must be set with `setDomain` and all `Data` objects added must be defined on the same domain. There is no restriction, however, on the `FunctionSpace` used.

setCycleAndTime(cycle, time)
sets the cycle and time values for this dataset. The cycle is an integer value which usually corresponds with the loop counter of the simulation script. That is, every time a new data file is created this counter is incremented. The value of `time` on the other hand is a floating point number that encodes some form of simulation time. Both, cycle and time may be read by analysis tools and shown alongside other metadata to the user.

setMeshLabels(x, y [, z=""])
sets the labels of the X, Y, and Z axis. By default, visualization tools display default strings such as "X-Axis" or "X" along the axes. Some export formats allow overriding these with more specific strings such as "Width", "Horizontal Distance", etc.

setMeshUnits(x, y [, z=""])
sets the units to be displayed along the X, Y, and Z axis in visualization tools (if supported). Not all export formats will use these values.

setMetadataSchemaString([schema="" [, metadata=""]])
adds custom metadata and/or XML schema strings to VTK files. The content of `schema` is added to the top-level *VTKFile* element so care must be taken to keep the resulting file valid. As an example, `schema` may contain the string `xmlns:gml="http://www.opengis.net/gml"`. The content of `metadata` will be written enclosed in `<MetaData>` tags. Thus, a valid example would be `<dataSource>something</dataSource>`. Note that these values are ignored by other exporters.

saveSilo(filename)
saves the dataset in the *SILO* file format to a file named `filename`. The file extension `.silo` will be automatically added if not present.

saveVTK(filename)
saves the dataset in the *VTK* file format to a file named `filename`. The file extension `.vtu` will be automatically added if not present. Certain combinations of function spaces cannot be written to a single *VTK* file due to format restrictions. In these cases this method will save separate files where each file contains compatible data. The function space name is appended to the filename to distinguish them.

8.2 Functions

createDataset(domain, **data)
creates an `EscriptDataset` object, sets its domain, populates it with the given `Data` objects and returns it. Note that it is not possible to set units for the data variables added with this function. If this is required, it is recommended to call this function with a domain only and use the `addData` method subsequently.

saveVTK(filename [, domain=None [, metadata="" [, metadata_schema=None]]], **data)
convenience function that creates a dataset with the given domain and `Data` objects and saves it to a file in the *VTK* file format. If `domain` is `None` the domain will be determined by the `Data` objects. See the `setDomain`, `addData`, `saveVTK`, and `setMetadataSchemaString` methods of the `EscriptDataset` class for details. Unlike the class method, the `metadata_schema` parameter should be a dictionary that maps namespace name to URI, e.g.
`{"gml":"http://www.opengis.net/gml"}`.

saveSilo(filename [, domain=None], **data)
convenience function that creates a dataset with the given domain and `Data` objects and saves it to a file in the *SILO* file format. If `domain` is `None` the domain will be determined by the `Data` objects. See the `setDomain`, `addData`, and `saveSilo` methods of the `EscriptDataset` class for details.

visitInitialize(simFile [, comment=""])
initializes the *VisIt* simulation interface which is responsible for the communication with a *VisIt* client. This function will create a file by the name given via `simFile` (extension `.sim2`) which can be loaded by a compatible *VisIt* client in order to connect to the simulation. The optional `comment` string is forwarded to the client. Note that this function only succeeds if *escript* was compiled with support for *VisIt* and the appropriate libraries are found in the runtime environment. Clients wanting to connect can only do so if the version number matches the version number used to compile `esys.weipa`. Calling this function does not make any data available yet, see the `visitPublishData` function.

visitPublishData(dataset)
publishes an `EscriptDataset` object through the *VisIt* simulation interface, checks for client requests and handles any outstanding ones. Before publishing any data, the `visitInitialize` function must

be called to set up the interface. Since this function not only publishes new data but polls for incoming connections and handles requests, it should be called as often as practical (even with the same dataset) to avoid timeout errors from clients. On the other hand it should be noted that the same process(es) deal with visualization requests that run your simulation. So a request for an expensive task by a *VisIt* client will pause the simulation code while it is being processed.

8.3 Visualizing *escript* Data

This section gives a very brief overview on how data exported through `esys.weipa` can be visualized. While there are many visualization packages available that are compatible with *VTK* and *SILO* files produced by *escript*, this discussion will refer to *VisIt* [34], an actively maintained open source package optimally suited to visualize and analyze large datasets both interactively and through *python* scripts. You can find a number of manuals, a wiki page and links to mailing lists on the *VisIt* website. It is assumed that you have a working *VisIt* installation that can be started by entering `visit` on the command line.

The examples that follow will use the output produced by the Elastic Deformation example from Section 1.4 (`heatedblock.py` in the example directory) which produces the file `deform.vtu`. This *VTK* file contains a 3D scalar variable called `stress` and a vector variable called `disp`, among others.

8.3.1 Using the *VisIt* GUI

Start the VisIt graphical user interface and open the file `deform.vtu` via the 'File' menu. Alternatively, you can directly open the file on startup by issuing

```
visit -o deform.vtu
```

You should see the *VisIt* GUI on the left hand side and an empty visualization window on the right. Click on 'Add' under Plots in the GUI to bring up a menu of plot types, then click on 'Pseudocolor' and select 'stress'. This will add a plot to the list which maps values of the 'stress' variable to colors. Note, that the plot will not be generated until you click on the 'Draw' button in the GUI. You should now see a coloured box in the visualization window which you can rotate around and inspect from different angles using your mouse. The example uses a coarse mesh of 10 by 10 by 10 elements which are clearly visible in this plot.

We can improve the visual effect by enabling interpolation between the elements. To do so, bring up the plot attributes by double-clicking the 'Pseudocolor - stress' plot entry in the GUI. Next, select 'Nodal' under 'Centering', click on 'Apply' and dismiss the dialog. Notice how the colours now smoothly blend into each other and the element boundaries are no longer visible.

Now we will add arrows to visualize the displacement vectors. Click on 'Add' and under 'Vector' select 'disp'. Once again click on 'Draw' to execute the new plot. By default only few vectors are shown but since the mesh is very coarse we can tell *VisIt* to draw all available vectors. Bring up the Vector plot attributes (double-click on the plot as before) and under 'Vector amount' select 'Stride', leaving the parameter as 1. Click on 'Apply' and dismiss the dialog.

As a final step we would like to see inside the plot. One possibility to do so is slicing. However, we want to keep all vectors while slicing only the Pseudocolor plot. In *VisIt* slicing is one of the Operators that may be added to plots and by default, Operators are added to *all* plots. To change this behaviour, uncheck the 'Apply operators to all plots' box which is located underneath the plot list in the GUI. Then select the Pseudocolor plot, bring up the Operators menu by clicking on 'Operators' and select 'ThreeSlice' from the 'Slicing' submenu. Again, click on 'Draw' to update the plots and notice how the box has now been sliced. We can move the slices to more suitable positions by editing the operator attributes. Click on the little triangle to the left of the Pseudocolor plot to reveal the list of elements that have been applied to it. Next, double-click the 'ThreeSlice' element to bring up the attribute window. Change the values to $X = 0.3$ and $Y = 0.3$, leaving $Z = 0$. Apply the changes and dismiss the dialog to see the result.

You can now create an image of the plots as shown in the window. First, adjust the save options to your needs in the 'Set Save options' dialog which is accessible from the 'File' menu. Then select 'Save Window' and you should find an image file with the name and location as entered in the options dialog.

8.3.2 Using the *VisIt* CLI (command line interface)

We will now perform exactly the same steps as in the last section but using the *python* interface of *VisIt* instead of the GUI. Start up the CLI by issuing

```
visit -cli
```

You should now see an empty visualization window but unlike in the previous section there will be no graphical user interface but a *python* command line instead. Enter the following commands, one by one, noticing the changes in the visualization window after every block of commands:

```
OpenDatabase("deform.vtu")
AddPlot("Pseudocolor","stress")
DrawPlots()

p=PseudocolorAttributes()
p.centering=p.Nodal
SetPlotOptions(p)

AddOperator("ThreeSlice")
DrawPlots()

t=ThreeSliceAttributes()
t.x=0.3
t.y=0.3
SetOperatorOptions(t)

AddPlot("Vector", "disp")
DrawPlots()

v=VectorAttributes()
v.useStride=1
SetPlotOptions(v)

s=SaveWindowAttributes()
#change settings as required
SaveWindow()
exit()
```

All but the last call to `DrawPlots()` is not required and was only put there for demonstrating the effects of the commands. You can save these commands to a file, e.g. `deformVis.py` and let *VisIt* process them non-interactively like so:

```
visit -cli -nowin -s deformVis.py
```

The `-nowin` option prevents the visualization window from being shown which is not required since the purpose of the script is to save an image file.

Obviously, we have barely touched on the powerful features of *VisIt* and this section was only meant to give you a minimal introduction. The *VisIt* website has a reference manual for the *python* interface that explains how to perform other operations programmatically, such as changing the view.

APPENDIX
A

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 involving tensors more compact by shortening and simplifying them.

There are two rules which make up the convention. Firstly, the rank of a 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 repeated subscripted variables, they are assumed to be summed over all possible values, from 0 to n. For example, the expression

$$y = a_0 b_0 + a_1 b_1 + \ldots + a_n b_n \tag{A.1}$$

can be represented as

$$y = \sum_{i=0}^{n} a_i b_i \tag{A.2}$$

then in Einstein notation:

$$y = a_i b_i \tag{A.3}$$

Another example:

$$\nabla p = \frac{\partial p}{\partial x_0}\mathbf{i} + \frac{\partial p}{\partial x_1}\mathbf{j} + \frac{\partial p}{\partial x_2}\mathbf{k} \tag{A.4}$$

can be expressed in Einstein notation as

$$\nabla p = p_{,i} \tag{A.5}$$

where the comma ',' in the subscript indicates the partial derivative.
For a tensor:

$$\sigma_{ij} = \begin{bmatrix} \sigma_{00} & \sigma_{01} & \sigma_{02} \\ \sigma_{10} & \sigma_{11} & \sigma_{12} \\ \sigma_{20} & \sigma_{21} & \sigma_{22} \end{bmatrix} \tag{A.6}$$

The δ_{ij} is the Kronecker δ-symbol, which is a matrix with ones in its diagonal entries ($i = j$) and zeros in the remaining entries ($i \neq j$).

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases} \tag{A.7}$$

APPENDIX
B

Changes from previous releases

3.2 to 3.2.1

- Improved documentation.
- domain_readers now work as does getFlux.
- More support for Dirac delta functions.
- Improvements to Darcy flow solvers (+coupled solvers not supported).
- Random data now drawn from boost::random on all platforms. Random data from intel's VSL is an option if building from source but the required sequence of MKL link instructions is left as an exercise for the reader.
- improved pythonicity:
  - __truediv__ and __rtruediv__ on esys.escript.Data
  - arithmetic operations on Data now return NotImplemented when they do not know what to do with their arguments.
  - unit tests do not call deprecated versions of assert??? methods.
- Various bug fixes.
- Code cleanup and warning removal.

3.1 to 3.2

- The deprecated name for the launcher has been removed. To run scripts use *run-escript* not *escript*.
- `esys.escript` is no longer automatically imported by importing `esys.finley`. You will need to import escript explicitly. (All of our example scripts do this anyway.)
- An experimental version of the new Dudley domain is now available.
- Various bug fixes and optimisations.
- New algorithms for gmsh support.
- Improvements to the AMG solver. AMG is the recommended solver for symmetric problems.
- Fixed compilation issues using netcdf.
- Redesigned configuration files to make it easier to compile from source without finding the locations of all your libraries.
- Faster rendering of documentation.

- Documentation is now hyperlinked.
- New data export module `esys.weipa`. The `saveVTK` functionality has been moved into this module, and while calling `saveVTK` from the `esys.escript` module still works it is discouraged and will be removed in a future release.
- New `esys.escript.DataManager` class for convenient checkpointing and exporting of escript data.
- *VisIt* simulation interface for online data access and visualization.
- Simpler interpolation and support for interpolation from 3D vectors.
- HRZ lumping has been added and some claification on how to use it.
- Data objects populated with "random" values can be created.

3.0 to 3.1

- The *escript* launcher has been renamed to *run-escript*. The old name will still work in this version but will be removed in the future.
- Lazy evaluation features have been improved and documented (see Section 2.5).
- The *escript* documentation now includes a new Cookbook which demonstrates how to solve sample problems using escript.
- Macro elements have been introduced.
- The `saveDataCSV` method allows one or more `Data` objects to be exported in CSV format (see Section 3.2.9).
- `Data` objects can be populated by interpolating from values in a table.
- The new `getInfLocator` and `getSupLocator` functions in `esys.escript.pdetools` return Locators to a minimal/maximal point over the data.
- There is a new class to model fault systems (`esys.escript.faultsystems.FaultSystem`).
- A beta version of an Algebraic Multigrid (AMG) solver is included.
- Inverting square matrices larger than 3x3 is now permitted if escript is compiled with Lapack support.
- If escript is compiled with a modern compiler, then inf/sup/Lsup will now report NaN, +/-inf as appropriate if those values appear in the data.
- Data.setTags will take tag names as well as tag numbers.
- The Scalar, Vector, Tensor, Tensor3, Tensor4 factory methods can now take arrays/nested sequence like objects as their initial values.
- escript.util.mkDir can now take a list of directories to create.
- Behind the scenes, *python* docstrings have been rewritten from epydoc to restructured text.
- Various other bug fixes and performance tweaks.

2.0 to 3.0

- The major change here was replacing `numarray` with `numpy`. For general instructions on converting scripts to use numpy see http://www.stsci.edu/resources/software_hardware/numarray/numarray2numpy.pdf. The specific changes to `esys.escript` are:
  - getValueOfDataPoint() which returned a `numarray`.array has been replaced by getTupleForDataPoint() which returns a *python* tuple containing the components of the data point. In the case of matrices or higher ranked data, the tuples will be nested. Use `numpy`.array(data.getTupleForDataPoint()) if a `numpy.ndarray` object is required.
  - getValueOfGlobalDataPoint() has similarly been replaced by getTupleForGlobalDataPoint().
  - `integrate(data)` now returns a `numpy.ndarray` instead of a `numarray`.array.

  Any python methods which previously accepted `numarray` objects now accept `numpy` objects instead.
- The way to define solver options for `LinearPDE` objects has changed. There is now a `SolverOptions` object attached to the `LinearPDE` object which handles the options of solvers used to solve the PDE. The following changes apply:
  - The `setTolerance` and `setAbsoluteTolerance` methods have been removed. Instead use `setTolerance` and `setAbsoluteTolerance` on the `SolverOptions` object. For example: `getSolverOptions().setTolerance(...)`
  - The `setSolverPackage` and `setSolverMethod` methods have been removed. Instead use the methods `setPackage`, `setSolverMethod` and `setPreconditioner`. For example: getSolverOptions().setPackage(...).
  - The static class variables defining packages, solvers and preconditioners have been removed and are now accessed via the corresponding static class variables in `SolverOptions`. For instance use `SolverOptions.PCG` instead of `LinearPDE.PCG` to select the preconditioned conjugate gradient method.
  - The `getSolution` now takes no argument. Use the corresponding methods of the `SolverOptions` object returned by `getSolverOptions()` to set values,
    e.g. use `getSolverOptions().setVerbosityOn()` instead of argument `verbose=True` and `getSolverOptions().setIterMax(1000)` instead of argument `iter_max=1000`.
- The `esys.pyvisi` module from previous releases has been deprecated and will no longer be supported. It is still present in the source code and can be used if you compile `esys.escript` from source. It will not be available in binary releases and its use is discouraged. *The documentation for `esys.pyvisi` is not available in this release.*

APPENDIX
C

Escript researchers and developers by release

	Releases	
Cihan Altinay	2.0	Current
Artak Amirbekyan	2.0	3.2
Joel Fenwick	2.0	Current
Lin Gao	2.0	Current
Lutz Gross	1.0	Current
Peter Hornby	1.0	2.0
Ken Steube	1.0	2.0
Elspeth Thorne	1.0	2.0
Matt Davies	1.0	2.0
Brett Tully	2.0	2.0
John Smilie	1.0	1.0
Cochrane	1.0	1.0
Rob Woodcock	1.0	2.0
Derek Hawcroft	1.0	2.0
Jon Gui	2.0	2.0

APPENDIX
D

Escript references

If you use escript in your research we would appreciate a citation (of course we do not require this). Possible references include:

```
@InProceedings{GROSS2010,
        author = {L. Gross and A. Amirbekyan and J. Fenwick and L. Gao
            and A. Mohajeri and H. M\"uhlhaus},
        title = {On lazy evaluation as a tool to optimize the
            efficiency of large scale numerical simulations in Python},
        booktitle = {ICCS 2010: Proceedings of the International
            Conference on Computational Science},
        pages = {2145--2153},
        year = {2010},
        editor = {Michael Blackman},
        publisher = {Elsevier}
        series = {Procedia Computer Science},
        month = {May},
        issn = {1877--0509},
        doi={doi:10.1016/j.procs.2010.04.240}
}
```

```
@InProceedings{lazyauspdc,
        author = {Joel Fenwick and Lutz Gross},
        title = {Lazy Evaluation of PDE Coefficients in the EScript System},
        booktitle = {Parallel and Distributed Computing 2010 (AusPDC2010)},
        pages = {71--76},
        year = {2010},
        editor = {Jinjun Chen and Rajiv Ranjan},
        volume = {107},
        series = {Conferences in Research and Practice in Information Technology},
        month = {January},
        issn = {1445--1336}
}
```

```
@article{GROSS2006,
        author = {L. Gross and L. Bourgouin and A. J. Hale and H.-B Muhlhaus},
        title = {Interface Modeling in Incompressible Media
        using Level Sets in Escript},
        journal = {Physics of the Earth and Planetary Interiors},
        year = 2007,
        volume = {163},
        pages = {23--34},
        month = {August},
        doi = {doi:10.1016/j.pepi.2007.04.004},
}
```

```
@article{GROSS2007,
        author = {L. Gross and B. Cumming and K. Steube and D. Weatherley},
        title = {A Python Module for PDE-Based Numerical Modelling},
        journal = {PARA},
        year = {2007},
        volume = {4699},
        pages = {270--279},
        doi = {doi:10.1007/978-3-540-75755-9},
        publisher = {Springer}
}
```

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