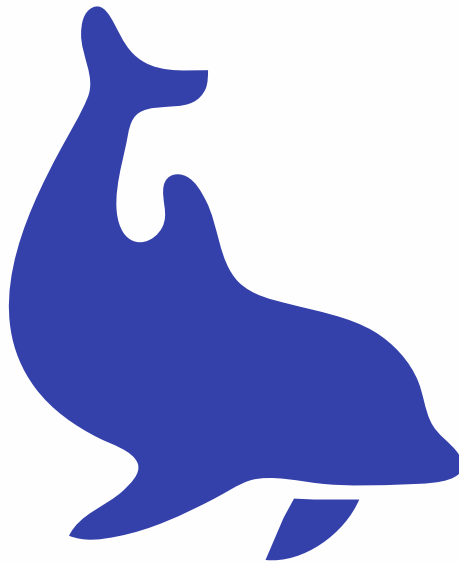


DOLFIN User Manual

October 4, 2005



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www.fenics.org

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Send comments and suggestions to dolfin-dev@fenics.org.

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About this manual

This manual is currently being written. A first version of this manual should be ready sometime in the fall of 2005.

Intended audience

This manual is written both for the beginning and the advanced user. There is also some useful information for developers. More advanced topics are treated at the end of the manual or in the appendix.

Typographic conventions

- Code is written in monospace (typewriter) **like this**.
- Commands that should be entered in a Unix shell are displayed as follows:

```
# ./configure
# make
```

Commands are written in the dialect of the **bash** shell. For other shells, such as **tcsh**, appropriate translations may be needed.

Enumeration and list indices

Throughout this manual, elements x_i of sets $\{x_i\}$ of size n are enumerated from $i = 0$ to $i = n - 1$. Derivatives in \mathbb{R}^n are enumerated similarly: $\frac{\partial}{\partial x_0}, \frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_{n-1}}$.

Contact

Comments, corrections and contributions to this manual are most welcome and should be sent to

`dolfin-dev@fenics.org`

Chapter 1

Introduction

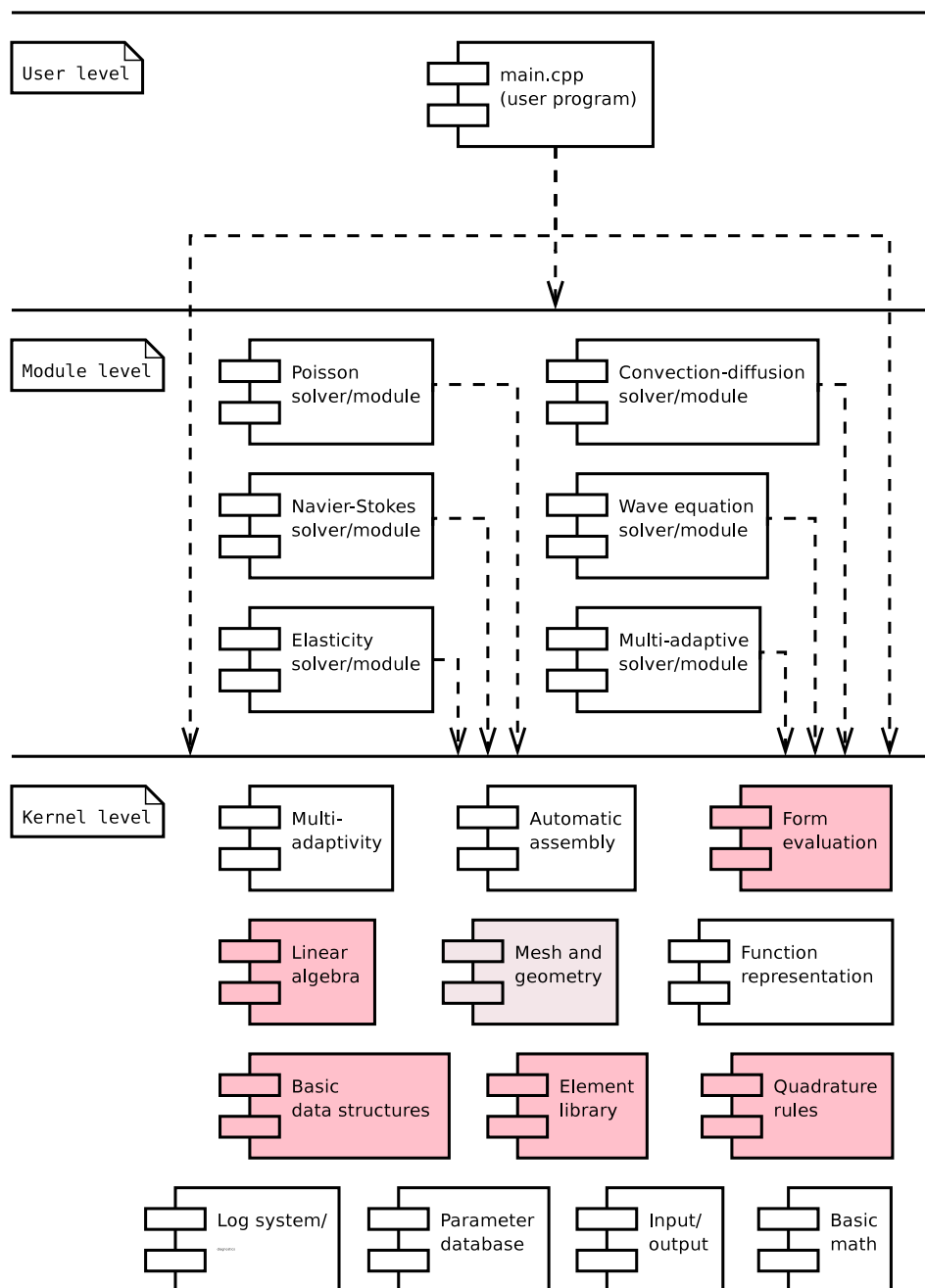
► *Developer's note:* This chapter is currently being written...

1.1 The FEniCS project

1.2 The finite element method

1.3 Overview

DOLFIN is implemented as a C++ library and can be used either as a stand-alone solver, or as a tool for the development and implementation of new methods. To simplify usage and emphasize structure, **DOLFIN** is organized into three levels of abstraction, referred to as *kernel level*, *module level*, and *user level*, as shown in Figure 1.1. Core features, such as the automatic evaluation of variational forms and adaptive mesh refinement, are implemented as basic tools at kernel level. At module level, new solvers/modules can be assembled from these basic tools and integrated into the system. At user level, a model of the form is specified and solved, either using one of the built-in solvers/modules or by direct usage of the basic tools.

Figure 1.1: Simplified component diagram of **DOLFIN**.

Chapter 2

Quickstart

This chapter demonstrates how to get started with **DOLFIN**, including downloading and installing the latest version of **DOLFIN**, and solving Poisson's equation. These topics are discussed in more detail elsewhere in this manual. In particular, see Appendix B for detailed installation instructions and Chapter 7 for a detailed discussion of how to solve partial differential equations with **DOLFIN**.

2.1 Downloading and installing DOLFIN

The latest version of **DOLFIN** can be found on the **FENICS** web page:

```
http://www.fenics.org/
```

The following commands illustrate the installation process, assuming that you have downloaded release 0.1.0 of **DOLFIN**:

```
# tar zxfv dolfin-0.1.0.tar.gz
# cd dolfin-0.1.0
# make
# make install
```

Note that you may need to be root on your system to do the last step. **DOLFIN** depends on a number of other packages, including the linear algebra package PETSc and the form compiler **FFC**. (See Appendix B for detailed instructions.)

2.2 Solving Poisson's equation with DOLFIN

Let's say that we want to solve Poisson's equation on the unit square $\Omega = (0, 1) \times (0, 1)$ with homogeneous Dirichlet boundary conditions on the boundary $\Gamma_0 = \{(x, y) \in \partial\Omega : x = 1\}$, homogeneous Neumann boundary conditions on the remaining part of the boundary and right-hand side given by $f = x \sin(y)$,

$$-\Delta u(x, y) = x \sin(y), \quad x \in \Omega = (0, 1) \times (0, 1), \quad (2.1)$$

$$u(x) = 0, \quad x \in \Gamma_0 = \{(x, y) \in \partial\Omega : x = 1\}, \quad (2.2)$$

$$\partial_n u(x) = 0, \quad x \in \partial\Omega \setminus \Gamma_0. \quad (2.3)$$

To solve a partial differential equation such as Poisson with **DOLFIN**, it must first be rewritten in *variational form*. The variational formulation of Poisson's equation reads: Find $u \in V$ such that

$$a(v, u) = L(v) \quad \forall v \in \hat{V}, \quad (2.4)$$

with (\hat{V}, V) a pair of suitable function spaces (the test and trial spaces). The bilinear form $a : \hat{V} \times V \rightarrow \mathbb{R}$ is given by

$$a(v, u) = \int_{\Omega} \nabla u \cdot \nabla v \, dx \quad (2.5)$$

and the linear form $L : \hat{V} \rightarrow \mathbb{R}$ is given by

$$L(v) = \int_{\Omega} f v \, dx. \quad (2.6)$$

2.2.1 Setting up the variational formulation

The variational formulation (2.4) must be given to **DOLFIN** as a pair of bilinear and linear forms (a, L) using the form compiler **FFC**. This is done by entering the definition of the forms in a text file with extension `.form`, e.g. `Poisson.form`, as follows:

```
element = FiniteElement('Lagrange', 'triangle', 1)

v = BasisFunction(element)
u = BasisFunction(element)
f = Function(element)

a = dot(grad(u), grad(v))*dx
L = f*v*dx
```

The example is given for piecewise linear finite elements in two dimensions, but other choices are available, including arbitrary order Lagrange elements in two and three dimensions.

To compile the pair of forms (a, L) , now call the form compiler on the command-line as follows:

```
# ffc Poisson.form
```

This generates the file `Poisson.h` which implements the forms in C++ for inclusion in your **DOLFIN** program.

2.2.2 Writing the solver

Having now compiled the variational formulation (2.4) with **FFC**, it is now easy to implement a solver for Poisson's equation. We first discuss the implementation line by line and then present the complete program. The source code for this example is available in the directory `src/demo/poisson/` of the **DOLFIN** source tree.

At the beginning of our C++ program, which we write in a text file named `main.cpp`, we must first include the header file `dolfin.h`, which gives our program access to the **DOLFIN** class library. In addition, we include the header file `Poisson.h` generated by the form compiler. Since all classes of the **DOLFIN** class library are defined within the namespace `dolfin`, we also specify that we want to work within this namespace:

```
#include <dolfin.h>
#include 'Poisson.h'

using namespace dolfin;
```

Next, we specify the right-hand side f of (2.1). This is done by defining a new subclass of `Function`, which we here will name `MyFunction`, and overloading the evaluation operator to return the value $f(x, y) = x \sin(y)$:

```
class MyFunction : public Function
{
    real operator() (const Point& p) const
    {
        return p.x*sin(p.y);
    }
};
```

The boundary condition is specified similarly, by overloading the evaluation operator for a subclass of `BoundaryCondition`:

```
class MyBC : public BoundaryCondition
{
    const BoundaryValue operator() (const Point& p)
    {
        BoundaryValue value;
        if ( std::abs(p.x - 1.0) < DOLFIN_EPS )
            value = 0.0;
        return value;
    }
};
```


We only need to specify the boundary condition explicitly on the Dirichlet boundary. On the remaining part of the boundary, **DOLFIN** assumes homogeneous Neumann boundary conditions by default.

Note that there is currently no easy way to impose non-homogeneous Neumann boundary conditions or other combinations of boundary conditions. This will most certainly be added to a future release of **DOLFIN**.

Since we are writing a C++ program, we need to create a `main` function. You are free to organize your program any way you like, but in this simple example we just write our program inside the `main` function:

```
int main()
{
    // Write your program here
    return 0;
}
```

The first thing we need to do is to create a mesh. **DOLFIN** relies on external programs for mesh generation, and imports meshes in **DOLFIN** XML format. However, for simple domains like the unit square or unit cube, **DOLFIN** provides a built-in mesh generator. To generate a uniform mesh of the unit square with mesh size $1/16$ (with a total of $2 \cdot 16^2 = 512$ triangles), we can just type

```
UnitSquare mesh(16, 16);
```

Next, we initialize the right-hand side, the boundary condition and the pair of forms that we have previously defined:

```
MyFunction f;
MyBC bc;
Poisson::BilinearForm a;
Poisson::LinearForm L(f);
```

All that remains is now to assemble the linear system $Ax = b$ representing the variational problem (2.4) and solve for the vector x . To assemble the system, we define a `Matrix A`, a `Vector b` and call the function `FEM::assemble()`:

```
Matrix A;
Vector x, b;
FEM::assemble(a, L, A, b, mesh, bc);
```

We may then solve the linear system $Ax = b$ for the degrees of freedom of the solution u using the GMRES method:

```
GMRES solver;
solver.solve(A, x, b);
```

Finally, we export the solution to a file for visualization. To do this, we define a `Function` which represents a field with given degrees of freedom in a function space defined by a mesh and a finite element, which we may obtain from the bilinear form by calling the member function `trial()`. Here, we choose to save the solution in Octave/MATLAB format, which we do by specifying a file name with extension `.m`:

```
Function u(x, mesh, a.trial());
File file('poisson.m');
file << u;
```

The complete program for Poisson's equation now looks as follows:

```
#include <dolfin.h>
#include "Poisson.h"

using namespace dolfin;

// Right-hand side
class MyFunction : public Function
{
  real operator() (const Point& p) const
  {
```

```
        return p.x*sin(p.y);
    }
};

// Boundary condition
class MyBC : public BoundaryCondition
{
    const BoundaryValue operator() (const Point& p)
    {
        BoundaryValue value;
        if ( std::abs(p.x - 1.0) < DOLFIN_EPS )
            value = 0.0;
        return value;
    }
};

int main()
{
    // Set up problem
    UnitSquare mesh(16, 16);
    MyFunction f;
    MyBC bc;
    Poisson::BilinearForm a;
    Poisson::LinearForm L(f);

    // Assemble linear system
    Matrix A;
    Vector x, b;
    FEM::assemble(a, L, A, b, mesh, bc);

    // Solve the linear system
    GMRES solver;
    solver.solve(A, x, b);

    // Save function to file
    Function u(x, mesh, a.trial());
    File file("poisson.m");
    file << u;

    return 0;
}
```

2.2.3 Compiling the program

The easiest way to compile the program is to create a `Makefile` that tells the standard Unix command `make` how to build the program. The following example shows how to write a `Makefile` for the above example:

```
CFLAGS = 'dolphin-config --cflags_dolphin'
LIBS    = 'dolphin-config --libs_dolphin'
CXX     = 'dolphin-config --compiler'

DEST    = dolphin-poisson
OBJECTS = main.o

all: $(DEST)

install:

clean:
    -rm -f *.o core *.core $(OBJECTS) $(DEST)

$(DEST): $(OBJECTS)
    $(CXX) -o $@ $(OBJECTS) $(CFLAGS) $(LIBS)

.cpp.o:
    $(CXX) $(CFLAGS) -c $<
```

With the `Makefile` in place, we just need to type `make` to compile the program, generating the executable as the file `dolphin-poisson`.

2.2.4 Running the program

To run the program, simply type the name of the executable:

```
# ./dolphin-poisson
Computing mesh connectivity:
Found 289 nodes
Found 512 cells
[...]
GMRES converged in 21 iterations.
```

```
Saved mesh mesh [...]
Saved function u [...]
```

2.2.5 Visualizing the solution

DOLFIN relies on external programs for visualization. In this example we chose to save the solution in Octave/MATLAB format, so we start Octave (or MATLAB) using the command `octave`. Then, in Octave, we import the solution and plot it using the `pdesurf` command:

```
octave:1> poisson
octave:2> pdesurf(points, cells, u)
```

Note that the commands `pdemesh`, `pdesurf` and `pdeplot` are not included with a standard installation of Octave, but are available in the subdirectory `src/utils/octave/` of the **DOLFIN** source tree.

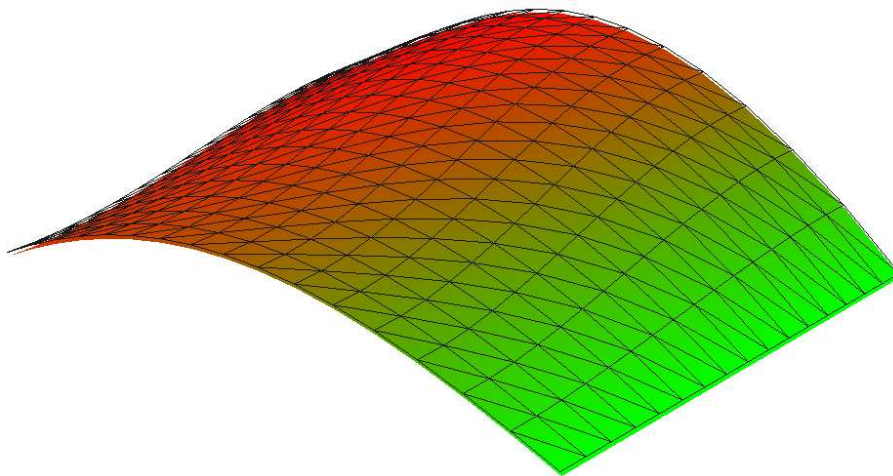


Figure 2.1: The solution of Poisson's equation (2.1) visualized in Octave.

Chapter 3

Linear algebra

DOLFIN does not have its own linear algebra routines, but instead use the external package PETSc [11] for linear algebra functionality.

PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It employs the MPI standard for all message-passing communication.

For convenience **DOLFIN** provide wrappers for some of the most common linear algebra functionality. For more advanced usage of PETSc, **DOLFIN** provide direct access to the PETSc pointers to be used with the standard PETSc interface.

3.1 Matrices and Vectors

The matrix class `Matrix` provides wrappers for initiating a sequential sparse matrix, or a sequential sparse matrix in block compressed row format. For parallel matrices one has to use the PETSc interface directly.

The code for initializing a sequential sparse $M \times N$ matrix take the form:

```
uint M = 100;
```

```
uint N = 100;  
Matrix A(M,N);
```

Similarly, the vector class `Vector` allows for a simple initialization of a M vector:

```
Vector b(M);
```

Further, wrappers for some basic functionality, such as matrix vector multiplication, norms etc., are provided with an intentionally simple interface, e.g. matrix vector multiplication:

```
Vector Ax;  
A.mult(b,Ax);
```

For more advanced operations, a pointer to the PETSc matrix and vector is accessed by `mat()` and `vec()` respectively.

3.2 Matrix-free matrices

The **DOLFIN** class `VirtualMatrix` represents a matrix-free matrix of dimension $M \times M$. The matrix-free matrix is a simple wrapper for a PETSc shell matrix. The interface is intentionally simple, and for advanced usage the PETSc `Mat` pointer is accessed by the function `mat()`.

The class `VirtualMatrix` enables the use of Krylov subspace methods for linear systems $Ax = b$, without having to explicitly store the matrix A . All that is needed is that the user-defined `VirtualMatrix` implements multiplication with vectors. Note that the multiplication operator needs to be defined in terms of PETSc data structures (`Vec`), since it will be called from PETSc.

3.3 Linear solvers

A general interface to all linear solvers for systems of the form $Ax = b$ is provided through the class `LinearSolver`.

In particular, wrappers for a direct LU solver and an iterative Krylov GMRES solver are implemented in the classes `LU` and `GMRES`.

To solve the linear system $Ax = b$ using GMRES in **DOLFIN**, we simply write:

```
Vec x;  
GMRES solver;  
solver.solve(A,x,b);
```

DOLFIN also provides a wrapper for an eigenvalue solver in PETSc. The following code computes the eigenvalues of the matrix A ,

```
Vector er, ec;  
EigenvalueSolver esolver;  
esolver.eigen(A,er,ec);
```

The real components of the eigenvalues are returned in the vector `er` and the complex components of the eigenvalues are returned in the vector `ec`. The procedure for computing the eigenvalues of a matrix is computationally intensive and should only be used for relatively small matrices.

3.4 Preconditioning

The `Preconditioner` class specifies the interface for user-defined Krylov method preconditioners. To implement our own preconditioner we only need to supply a function that approximately solves the linear system given a right-hand side.

As a complement to PETSc, **DOLFIN** also uses Hypre [3], which is a library for solving large, sparse linear systems of equations on massively parallel computers.

To use a preconditioner from Hypre with our PETSc solver in **DOLFIN**, we write:

```
PCSetType(PC pc, PCHYPRE );  
PCHYPRESetType(PC pc, "boomeramg");
```

In particular, the above preconditioner `boomeramg` is an algebraic multigrid preconditioner, which is very useful.

Chapter 4

Functions

► *Developer's note:* This chapter is currently being written...

A function in **DOLFIN** is represented by the class `Function`, and is either scalar or vector-valued. There are two type of functions in **DOLFIN**; functions which belong to the finite element space and user-defined functions. Both of these types of functions are discussed in this chapter.

4.1 Functions in the finite element space

A function in the finite element space is defined in terms of a finite element, a mesh and a vector containing the value of the function at a finite number of points (nodal points). For example, a scalar function u in two dimensions is given by:

$$u(x, y) = \sum_{i=1}^N \varphi_i(x, y) u_i, \quad (4.1)$$

where φ_i is the finite element shape function (basis function) associated with node i , u_i is the value of the function u at node i and N is the number of nodes.

4.1.1 Intializing functions

A function can be initialized in several ways. An empty function `u` is initialized by:

```
Function u;
```

A function can also be created by:

```
Vector x;  
Function u(x);
```

in which case the function is defined in terms of the vector `x` which contains the terms u_i . **DOLFIN** will then choose the mesh and the finite element type automatically, which are necessary to define the basis functions $\{\varphi_i\}_{i=1}^N$. Creating a function with the code:

```
Vector x;  
Mesh mesh;  
Function u(x,mesh);
```

leads to a function `u` which is defined in terms of the vector `x` and the mesh `mesh`. **DOLFIN** will select the finite element automatically. Finally, creating a function by

```
Vector x;  
Mesh mesh;  
FiniteElement element;  
Function u(x,mesh,element);
```

leads to a function `u` which is defined in terms of the vector `x`, the mesh `mesh` and the finite element `element`.

After a function has been initialized, it is possible to associate a finite element using the function `set`. For example,

```
Vector x;  
Mesh mesh;  
FiniteElement element;  
  
Function u(x,mesh);  
u.set(element);
```

Usually, the finite element is given by the bilinear form defining the problem. Considering the Poisson example in Chapter 2), a function `u` can be defined by:

```
Vector x;  
Mesh mesh;  
FiniteElement element;  
  
Poisson::BilinearForm a;  
element = a.trial();  
  
Function u(x,mesh);  
u.set(element);
```

The trial (basis) functions associated with the bilinear form `a` have been used to define this function.

4.1.2 Retrieving function details

It is possible to find out with which vector, mesh and finite element a function is defined. Given a function `u`, the associated vector, mesh and finite element can be returned by:

```
Vector x;  
Mesh mesh;  
FiniteElement element;
```

```
x      = u.vector();  
mesh   = u.mesh();  
element = u.element();
```

4.1.3 Evaluating functions

Functions can be output in various file formats which are examined in detail in Chapter 8.

4.2 User-defined functions

A user defined function is a function in terms of the spatial coordinates and possibly time. They are typically used for defining source terms and initial conditions. For example, a source could be given by

$$f = f(x, y, z) = yz \sin(x/\pi). \quad (4.2)$$

4.3 Time-dependent functions

Time-dependent and pseudo time-dependent functions.

Chapter 5

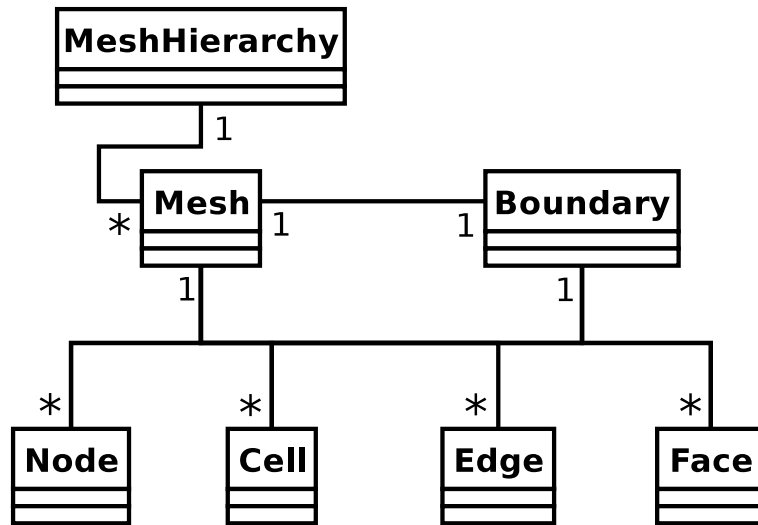
The mesh

► *Developer's note:* This chapter is currently being written...

The concept of a *mesh* is central in the implementation of adaptive Galerkin finite element methods for partial differential equations. Other important concepts include *nodes*, *cells*, *edges*, *faces*, *boundaries*, and *mesh hierarchies*. These concepts are all implemented as C++ classes in **DOLFIN**, as shown in Figure 5.1.

Algorithms operating on a mesh, including adaptive mesh refinement, can often be expressed in terms of *iterators*, i.e., objects used for the traversal of aggregate structures, such as the list of nodes contained in a mesh. Iterators implemented in **DOLFIN** include a `NodeIterator`, `CellIterator`, `EdgeIterator`, `FaceIterator`, and a `MeshIterator`. Table 5.1 provides an example of a code that displays all node neighbors of all nodes of all cells within a given mesh.

Adaptive mesh refinement is implemented in **DOLFIN** for triangular meshes (in 2D) and tetrahedral meshes (in 3D), see Figure 5.2, based on the algorithm given in [14]. To refine a mesh, the cells (triangles or tetrahedrons) are first marked according to some criterion for refinement, before the mesh is refined. A hierarchy of meshes, that can be used for example in a multigrid computation, is automatically created.

Figure 5.1: Class diagram of the basic mesh classes in **DOLFIN**.

```

for (CellIterator c(m); !c.end(); ++c)
  for (NodeIterator n1(c); !n1.end(); ++n1)
    for (NodeIterator n2(n1); !n2.end(); ++n2)
      cout << *n2 << endl;

```

Table 5.1: Iteration over all node neighbors $n2$ of the nodes $n1$ within all cells c of the mesh m .

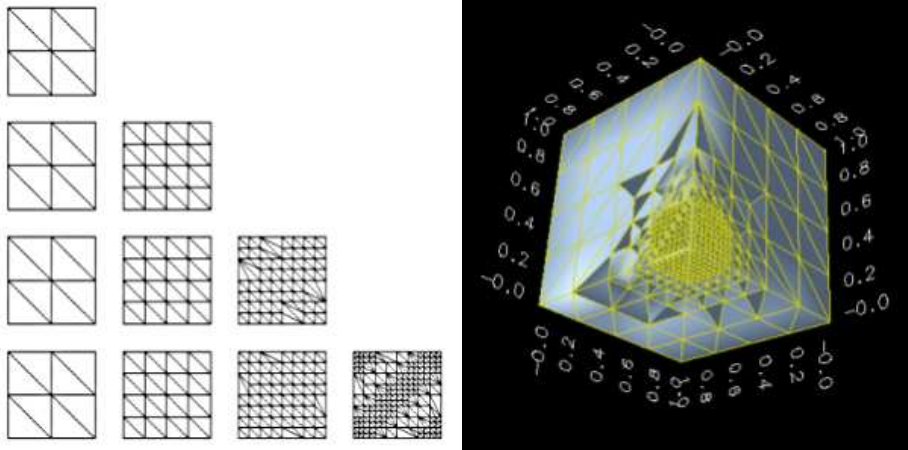


Figure 5.2: Adaptive mesh refinement of triangular and tetrahedral meshes in **DOLFIN**.

```
// Mark cells for refinement
for (CellIterator cell(mesh); !cell.end(); ++cell)
    if ( ... )
        cell->mark();

// Refine mesh
mesh.refine();
```

Table 5.2: Sketch of adaptive mesh refinement in **DOLFIN**.

Chapter 6

Ordinary differential equations

► *Developer's note:* This chapter is currently being written...

Chapter 7

Partial differential equations

7.1 Boundary value problems

As a prototype of a boundary value problem in \mathbb{R}^d we consider the scalar Poisson equation with homogeneous Dirichlet boundary conditions

$$\begin{aligned} -\Delta u(x) &= f(x) & x \in \Omega \subset \mathbb{R}^d \\ u(x) &= 0 & x \in \partial\Omega. \end{aligned} \tag{7.1}$$

7.2 Variational formulation

A variational formulation of (7.1) take the form: find $u \in V$ such that

$$a(v, u) = L(v) \quad \forall v \in \hat{V}, \tag{7.2}$$

where $a(\cdot, \cdot) : \hat{V} \times V \rightarrow \mathbb{R}$ is a bilinear form acting on $\hat{V} \times V$, with \hat{V} and V the *test space* and *trial space* respectively, defined by

$$a(v, u) = \int_{\Omega} \nabla v \cdot \nabla u \, dx = \int_{\Omega} \frac{\partial v}{\partial x_i} \frac{\partial u}{\partial x_i} \, dx, \tag{7.3}$$

where we employ tensor notation so that the double index i means summation from $i = 1, \dots, d$, and $L(\cdot) : \hat{V} \rightarrow \mathbb{R}$ is a linear form acting on the test space \hat{V} , defined by

$$L(v) = \int_{\Omega} f v \, dx. \quad (7.4)$$

For this problem we typically use $V = \hat{V} = H_0^1(\Omega)$, with $H_0^1(\Omega)$ the standard Sobolev space of square integrable functions with also their first derivatives square integrable (in the Lebesgue sense), with the functions being zero on the boundary (in the sense of traces).

The Finite Element Method FEM for (7.2) is now: find $U \in V_h$ such that

$$a(v, U) = L(v) \quad \forall v \in \hat{V}_h, \quad (7.5)$$

where $V_h \subset V$ and $\hat{V}_h \subset \hat{V}$ are finite dimensional subspaces of dimension N . The finite element spaces V_h, \hat{V}_h are characterized by their sets of basis functions $\{\varphi_i\}_{i=1}^N, \{\hat{\varphi}_i\}_{i=1}^N$, and thus the FEM method (7.5) is specified by the variational form and the basis functions of V_h and \hat{V}_h .

7.3 Finite elements and FIAT

Finite element basis functions in **DOLFIN** are defined using **FIAT**, which supports the generation of arbitrary order Lagrange finite elements on lines, triangles, and tetrahedra. Upcoming versions of **FIAT** will also support Hermite and nonconforming elements as well as H(div) and H(curl) elements such as Raviart-Thomas and Nedelec.

7.4 Compiling the variational form with FFC

In **DOLFIN** a PDE is defined in variational form using tensor notation in a `.form` file, which is compiled using the *FEniCS Form Compiler* **FFC**.

In the language of **FFC**, with $V_h = \hat{V}_h$ the space of piecewise linear Lagrange finite elements on a tetrahedral mesh, (7.5) is defined as:

```
element = FiniteElement("Lagrange", "tetrahedron", 1)

v = BasisFunction(element)
u = BasisFunction(element)
f = Function(element)

a = v.dx(i)*u.dx(i)*dx
L = v*f*dx
```

where `*dx` signifies integration over the domain Ω , and the finite element space is constructed using **FIAT**. **DOLFIN** is not communicating directly with **FIAT**, but only through **FFC** in the definition of the variational form in the `.form` file.

Compiling the file with

```
# ffc Poisson.form
```

generates a file `Poisson.h`, containing classes for the bilinear form $a(\cdot, \cdot)$ and the linear form $L(\cdot)$, and classes for the finite element spaces V_h and \hat{V}_h .

7.5 Element matrices and vectors

The element matrices and vectors for a given cell may be factored into two tensors, with one tensor depending on the geometry of the cell, and the other tensor only involving integration of products of basis functions and their derivatives over the reference element.

For efficiency in the computation of the element matrices and vectors, **FFC** precomputes the tensors that are independent of the geometry of a certain cell.

7.6 Assemble matrices and vectors

The class `FEM` automates the assembly algorithm, constructing a linear system of equations from a given PDE, given in the form of a variational problem (7.2), with a bilinear form $a(\cdot, \cdot)$ and a linear form $L(\cdot)$.

The classes `BilinearForm` and `LinearForm` are automatically generated by **FFC**, and to assemble the corresponding matrix and vector for the Poisson problem (7.2) with source term f , we write:

```
Poisson::BilinearForm a;  
Poisson::LinearForm L(f);  
  
Mesh mesh;  
Mat A;  
Vec b;  
  
FEM::assemble(a,L,A,b,mesh);
```

In the `assemble()` function the element matrices and vectors are computed by calling the function `eval()` in the classes `Bilinearform` and `Linearform`. The `eval()` functions at a certain element in the assembly algorithm take as argument an `AffineMap` object, describing the mapping from the reference element to the actual element, by computing the jacobian J of the mapping (also J^{-1} and $\det(J)$ are computed).

7.7 Specifying boundary conditions and data

The boundary conditions are specified by defining a new subclass of the class `BoundaryCondition`, which we here will name `MyBC`:

```
class MyBC : public BoundaryCondition  
{  
    const BoundaryValue operator() (const Point& p)
```



```

{
    BoundaryValue value;
    if ( std::abs(p.x - 0.0) < DOLFIN_EPS ) value = 0.0;
    if ( std::abs(p.x - 1.0) < DOLFIN_EPS ) value = 0.0;
    if ( std::abs(p.y - 0.0) < DOLFIN_EPS ) value = 0.0;
    if ( std::abs(p.y - 1.0) < DOLFIN_EPS ) value = 0.0;
    if ( std::abs(p.z - 0.0) < DOLFIN_EPS ) value = 0.0;
    if ( std::abs(p.z - 1.0) < DOLFIN_EPS ) value = 0.0;
    return value;
}
};

```

where we have assumed homogeneous Dirichlet boundary conditions for the unit cube. We only need to specify the boundary condition explicitly on the Dirichlet boundary. On the remaining part of the boundary, **DOLFIN** assumes homogeneous Neumann boundary conditions by default.

The boundary condition is then imposed as an argument for the `assemble()` function.

```

MyBC bc;
FEM::assemble(a,L,A,b,mesh,bc);

```

There is currently no easy way to impose non-homogeneous Neumann boundary conditions or other combinations of boundary conditions. This will be added to a future release of **DOLFIN**.

The right-hand side f of (7.1) is similarly specified by defining a new subclass of `Function`, which we here will name `MyFunction`, and overloading the evaluation operator:

```

class MyFunction : public Function
{
    real operator() (const Point& p) const
    {
        return p.x*p.z*sin(p.y);
    }
}

```

$$\left. \begin{array}{l} \end{array} \right\} \\ \};$$

with the source $f(x, y, z) = xz \sin(y)$.

7.8 Initial value problems

semidiscretization, space-time FEM,

Chapter 8

Input/output

DOLFIN relies on external programs for pre- and post-processing, which means that computational meshes must be imported from file (pre-processing) and computed solutions must be exported to file and then imported into another program for visualization (post-processing). To simplify this process, **DOLFIN** provides support for easy interaction with files and includes output formats for a number of visualization programs.

8.1 Files and objects

A file in **DOLFIN** is represented by the class `File` and reading/writing data is done using the standard C++ operators `>>` (read) and `<<` (write).

Thus, if `file` is a `File` and `object` is an object of some class that can be written to file, then the object can be written to file as follows:

```
file << object;
```

Similarly, if `object` is an object of a class that can be read from file, then data can be read from file (overwriting any previous data held by the object) as follows:

```
file >> object;
```

The format (type) of a file is determined by its filename suffix, if not otherwise specified. Thus, the following code creates a **File** for reading/writing data in **DOLFIN** XML format:

```
File file('data.xml');
```

A complete list of file formats and corresponding file name suffixes is given in Table 8.1.

Alternatively, the format of a file may be explicitly defined. One may thus create a file named `data.xml` for reading/writing data in GNU Octave format:

```
File file('data.xml', File::octave);
```

Suffix	Format	Description
.xml/.xml.gz	File::xml	DOLFIN XML
.pvd	File::vtk	VTK
.dx	File::opendx	OpenDX
.m	File::octave	GNU Octave
(.m)	File::matlab	MATLAB
.tec	File::tecplot	Tecplot
.msh/.res	File::gid	GiD

Table 8.1: File formats and corresponding file name suffixes.

Although many of the classes in **DOLFIN** support file input/output, it is not supported by all classes and the support varies with the choice of file format. A summary of supported classes/formats is given in Table 8.2.

► *Developer's note:* Some of the file formats are partly broken after changing the linear algebra backend to PETSc. (Do `grep FIXME` in `src/kernel/io/`.)

Format	Vector	Matrix	Mesh	Function	Sample
File::xml	in/out	in/out	in/out	—	—
File::vtk	—	—	out	out	—
File::opendx	—	—	out	out	—
File::octave	out	out	out	out	out
File::matlab	out	out	out	out	out
File::tecplot	—	—	out	out	—
File::gid	—	—	out	out	—

Table 8.2: Matrix of supported combinations of classes and file formats for input/output in **DOLFIN**.

8.2 File formats

In this section, we give some pointers to each of the file formats supported by **DOLFIN**. For detailed information, we refer to the respective user manual of each format/program.

► *Developer's note:* This section needs to be improved and expanded. Any contributions are welcome.

8.2.1 DOLFIN XML

DOLFIN XML is the native format of **DOLFIN**. As the name says, data is stored in XML ASCII format. This has the advantage of being a robust and human-readable format, and if the files are compressed there is little overhead in terms of file size compared to a binary format.

DOLFIN automatically handles gzipped XML files, as illustrated by the following example which reads a **Mesh** from a compressed **DOLFIN** XML file and saves the mesh to an uncompressed **DOLFIN** XML file:

```
Mesh mesh;
```

```
File in('mesh.xml.gz');
in >> mesh;

File out('mesh.xml');
out << mesh;
```

The same thing can of course be accomplished by

```
# gunzip -c mesh.xml.gz > mesh.xml
```

on the command-line.

There is currently no visualization tool that can read **DOLFIN** XML files, so the main purpose of this format is to save and transfer data.

8.2.2 VTK

Data saved in VTK format [13] can be visualized using various packages. The powerful and freely available ParaView [10] is recommended. Alternatively, VTK data can be visualized in MayaVi [5], which is recommended for quality vector PostScript output. Time-dependent data is handled automatically in the VTK format.

The below code illustrates how to export a function in VTK format:

```
Function u;

File out('data.pvd');
out << u;
```

The sample code produces the file `data.pvd`, which can be read by ParaView. The file `data.pvd` contains a list of files which contain the results computed by **DOLFIN**. For the above example, these files would be named `dataXXX.vtu`, where `XXX` is a counter which is incremented each time the function is saved. If the function `u` was to be saved three times, the files

```
data000000.vtu  
data000001.vtu  
data000002.vtu
```

would be produced. Individual snapshots can be visualized by opening the desired file with the extension `.vtu` using ParaView.

ParaView can produce on-screen animations. High quality animations in various formats can be produced using a combination of ParaView and MEncoder [6].

► *Developer's note:* Add MEncoder example to create animation.

8.2.3 OpenDX

OpenDX [9] is a powerful free visualization tool based on IBM's *Visualization Data Explorer*. To visualize data with OpenDX, a user needs to build a *visual program* that instructs OpenDX how to extract and visualize relevant parts of your data. **DOLFIN** provides a ready-made visual program suitable for visualization of **DOLFIN** data in OpenDX. The visual program can be found in the subdirectory `src/utils/opendx/` of the **DOLFIN** source tree (file `dolfin.net` and accompanying configuration `dolfin.cfg`).

8.2.4 GNU Octave

GNU Octave [7] is a free clone of MATLAB that can be used to visualize solutions computed in **DOLFIN**, using the commands `pdemesh`, `pdesurf` and `pdeplot`. These commands are normally not part of GNU Octave but are provided by **DOLFIN** in the subdirectory `src/utils/octave/` of the **DOLFIN** source tree. These commands require the external program `ivview` included in the open source distribution of Open Inventor [8]. (Debian users install the package `inventor-clients`.)

To visualize a solution computed with **DOLFIN** and exported in GNU Octave format, first load the solution into GNU Octave by just typing the name of

the file without the `.m` suffix. If the solution has been saved to the file `poisson.m`, then just type

```
octave:1> poisson
```

The solution can now be visualized using the command

```
octave:2> pdesurf(points, cells, u)
```

or to visualize just the mesh, type

```
octave:3> pdesurf(points, edges, cells)
```

8.2.5 MATLAB

Since MATLAB [4] is not free, users are encouraged to use GNU Octave whenever possible. That said, data is visualized in much the same way in MATLAB as in GNU Octave, using the MATLAB commands `pdemesh`, `pdesurf` and `pdeplot`.

8.2.6 Tecplot

Tecplot [12] is a proprietary visualization tool. The Tecplot format is not actively maintained and may be removed in future versions of **DOLFIN** (if there is not sufficient interest to maintain the format).

8.2.7 GiD

GiD [2] is a proprietary visualization tool. The GiD format is not actively maintained and may be removed in future versions of **DOLFIN** (if there is not sufficient interest to maintain the format).

8.3 A note on new file formats

With some effort, **DOLFIN** can be expanded with new file formats. Any contributions are welcome. If you wish to contribute to **DOLFIN**, then adding a new file format (or improving upon an existing file format) is a good place to start. Take a look at one of the current formats in the subdirectory `src/kernel/io/` of the **DOLFIN** source tree to get a feeling for how to design the file format, or ask at `dolfin-dev@fenics.org` for directions.

Chapter 9

The log system

DOLFIN provides provides a simple interface for uniform handling of log messages, including warnings and errors. All messages are collected to a single stream, which allows the destination and formatting of the output from an entire program, including the **DOLFIN** library, to be controlled by the user.

9.1 Generating log messages

Log messages can be generated using the function `dolfin_info()` available in the `dolfin` namespace:

```
void dolfin_info(const char *message, ...);
```

which works similarly to the standard C library function `printf`. The following examples illustrate the usage of `dolfin_info()`:

```
dolfin_info("Solving linear system.");  
dolfin_info("Size of vector: %d.", x.size());  
dolfin_info("R = %.3e (TOL = %.3e)", R, TOL);
```

As an alternative to `dolfin.info()`, **DOLFIN** provides a C++ style interface to generating log messages. Thus, the above examples can also be implemented as follows:

```
cout << "Solving linear system." << endl;
cout << "Size of vector: " << x.size() << "." << endl;
cout << "R = " << R << " (TOL = " << TOL << ")" << endl;
```

Note the use of `dolfin::cout` and `dolfin::endl` from the `dolfin` namespace, corresponding to the standard `std::cout` and `std::endl` in namespace `std`. If log messages are directed to standard output (see below), then `dolfin::cout` and `std::cout` may be mixed freely.

Most classes provided by **DOLFIN** can be used together with `dolfin::cout` and `dolfin::endl` to display short informative messages about objects:

```
Matrix A(10, 10);
cout << A << endl;
```

To display detailed information for an object, use the member function `disp()`:

```
Matrix A(10, 10);
A.disp();
```

Use with caution for large objects. For a `Matrix`, calling `disp()` will display all matrix entries.

9.2 Warnings and errors

Warnings and error messages can be generated using the macros

```
dolfin_warning(message);
dolfin_error(message);
```

In addition to displaying the given string message, the macro `dolfin_error()` also displays information about the location of the code that generated the error (file, function name and line number). Once an error is encountered, the program is stopped.

Note that in order to pass formatting strings and additional arguments to warnings or errors, the variations `dolfin_error1()`, `dolfin_error2()` and so on must be used, as illustrated by the following examples:

```
dolfin_error("GMRES solver did not converge.");
dolfin_error1("Unable to find face opposite to node %d.", n);
dolfin_error2("Unable to find edge between nodes %d and %d.", n0, n1);
```

9.3 Debug messages and assertions

The macro `dolfin_debug()` works similarly to `dolfin_info()`:

```
dolfin_debug(message);
```

but in addition to displaying the given message, information is printed about the location of the code that generated the debug message (file, function name and line number).

Note that in order to pass formatting strings and additional arguments with debug messages, the variations `dolfin_debug1()`, `dolfin_debug2()` and so on, depending on the number of arguments, must be used.

Assertions can often be a helpful programming tool. Use assertions whenever you assume something about a variable in your code, such as assuming that given input to a function is valid. **DOLFIN** provides the macro `dolfin_assert()` for creating assertions:

```
dolfin_assert(check);
```

This macro accepts a boolean expression and if the expression evaluates to false, an error message is displayed, including the file, function name and

line number of the assertion, and a segmentation fault is raised (to enable easy attachment to a debugger). The following examples illustrate the use of `dolfin_assert()`:

```
dolfin_assert(i >= 0);  
dolfin_assert(i < n);  
dolfin_assert(cell.type() == Cell::triangle);  
dolfin_assert(cell.type() == Cell::tetrahedron);
```

Note that assertions are only active when compiling **DOLFIN** and your program with `DEBUG` defined (configure option `--enable-debug` or compiler flag `-DDEBUG`). Otherwise, the macro `dolfin_assert()` expands to nothing, meaning that liberal use of assertions does not affect performance, since assertions are only present during development and debugging.

9.4 Task notification

The two functions `dolfin_begin()` and `dolfin_end()` available in the `dolfin` name space can be used to notify the **DOLFIN** log system about the beginning and end of a task:

```
void dolfin_begin();  
void dolfin_end();
```

Alternatively, a string message (or a formatting string with optional arguments) can be supplied:

```
void dolfin_begin(const char* message, ...);  
void dolfin_end(const char* message, ...);
```

These functions enable the **DOLFIN** log system to display messages, warnings and errors hierarchically, by automatically indenting the output produced between calls to `dolfin_begin()` and `dolfin_end()`. A program may contain an arbitrary number of nested tasks.

9.5 Progress bars

The **DOLFIN** log system provides the class `Progress` for simple creation of progress sessions. A progress session automatically displays the progress of a computation using a progress bar.

If the number of steps of a computation is known, a progress session should be defined in terms of the number of steps and updated in each step of the computation as illustrated by the following example:

```
Progress p('Assembling', mesh.noCells());
for (CellIterator c(mesh); !c.end(); ++c)
{
    ...
    p++;
}
```

It is also possible to specify the step number explicitly by assigning an integer to the progress session:

```
Progress p('Iterating over vector', x.size())
for (uint i = 0; i < x.size(); i++)
{
    ...
    p = i;
}
```

Alternatively, if the number of steps is unknown, the progress session needs to be updated with the current percentage of the progress:

```
Progress p('Time-stepping');
while ( t < T )
{
    ...
    p = t / T;
}
```

The progress bar created by the progress session will only be updated if the progress has changed significantly since the last update (by default at least 10%). The amount of change needed for an update can be controlled using the parameter ‘‘progress step’’:

```
dolphin_set(‘‘progress step’’, 0.01);
```

Note that several progress sessions may be created simultaneously, or nested within tasks.

9.6 Controlling the destination of output

By default, the **DOLFIN** log system directs messages to standard output (the terminal). Other options include directing messages to a curses interface or turning of messages completely. To specify the output destination, use the function `dolphin_output()` available in the `dolphin` namespace:

```
void dolphin_output(const char* destination);
```

where `destination` is one of ‘‘plain text’’ (standard output), ‘‘curses’’ (curses interface) or ‘silent’’ (no messages printed).

When messages are directed to the **DOLFIN** curses interface, a text-mode graphical and interactive user-interface is started in the current terminal window. To see a list of options, press ‘h’ for help. The curses-interface is updated periodically but the function `dolphin_update()` can be used to force a refresh of the display.

It is possible to switch the **DOLFIN** log system on or off using the function `dolphin_log()` available in the `dolphin` namespace. This function accepts as argument a `bool`, specifying whether or not messages should be directed to the current output destination. This function can be useful to suppress excessive logging, for example when calling a function that generates log messages multiple times:


```
GMRES gmres;
while ( ... )
{
    ...
    dolfin_log(false);
    gmres.solve(A, x, b);
    dolfin_log(true);
    ...
}
```


Chapter 10

Parameters

DOLFIN keeps a global database of parameters that control the behavior of the various components of **DOLFIN**. Parameters are controlled using a uniform type-independent interface that allows retrieving the values of existing parameters, modifying existing parameters and adding new parameters to the database.

10.1 Retrieving the value of a parameter

To retrieve the value of a parameter, use the function `dolfin_get()` available in the `dolfin` namespace:

```
Parameter dolfin_get(const char* key);
```

This function accepts as argument a string `key` and returns the value of the parameter matching the given key. An error message is printed through the log system if there is no parameter with the given key in the database.

The value of the parameter is automatically cast to the correct type when assigning the value of `dolfin_get()` to a variable, as illustrated by the following examples:

```
real TOL = dolfin_get('tolerance');
int num_samples = dolfin_get('number of samples');
bool solve_dual = dolfin_get('solve dual problem');
std::string filename = dolfin_get('file name');
```

Note that there is a cost associated with accessing the value of a parameter, so if the value of a parameter is to be used multiple times, then it should be retrieved once and stored in a local variable as illustrated by the following example:

```
int num_samples = dolfin_get('number of samples');
for (int i = 0; i < num_samples; i++)
{
    ...
}
```

10.2 Modifying the value of a parameter

To modify the value of a parameter, use the function `dolfin_set()` available in the `dolfin` namespace:

```
void dolfin_set(const char* key, ...);
```

This function accepts as arguments a string `key` together with the corresponding value. The value type should match the type of parameter that is being modified. An error message is printed through the log system if there is no parameter with the given key in the database.

The following examples illustrate the use of `dolfin_set()`:

```
dolfin_set('tolerance', 0.01);
dolfin_set('number of samples', 10);
dolfin_set('solve dual problem', true);
dolfin_set('file name', 'solution.xml');
```

Note that changing the values of parameters using `dolfin_set()` does not change the values of already retrieved parameters; it only changes the values of parameters in the database. Thus, the value of a parameter must be changed before using a component that is controlled by the parameter in question.

10.3 Adding a new parameter

To add a parameter to the database, use the function `dolfin_parameter()` available in the `dolfin` namespace:

```
void dolfin_parameter(Parameter::Type type,
                      const char* key, ...);
```

This function accepts three arguments: the type of the new parameter, a unique key identifying the new parameter and the value of the new parameter.

Possible values for `type` are

- `Parameter::REAL`, corresponding to `real`;
- `Parameter::INT`, corresponding to `int`;
- `Parameter::BOOL`, corresponding to `bool`;
- `Parameter::STRING`, corresponding to `std::string`.

The following examples illustrate the use of `dolfin_parameter()`:

```
dolfin_parameter(Parameter::REAL, 'tolerance', 0.01);
dolfin_parameter(Parameter::INT, 'number of samples', 10);
dolfin_parameter(Parameter::BOOL, 'solve dual problem', true);
dolfin_parameter(Parameter::STRING, 'file name', 'solution.xml');
```

10.4 Saving parameters to file

To save the current database of parameters to a file in **DOLFIN** XML format, use the function `dolfin_save()` available in the `dolfin` namespace:

```
void dolfin_save(const char* filename);
```

When running a simulation in **DOLFIN**, saving the parameter database to a file is an easy way to document the set of parameters used in the simulation.

10.5 Loading parameters from file

To load a set of parameters from a file into the parameter database, use the function `dolfin_load()` available in the `dolfin` namespace:

```
void dolfin_load(const char* filename);
```

This function accepts as argument the name of a file containing a list of parameters in **DOLFIN** XML format, as illustrated below:

```
<?xml version='1.0' encoding='UTF-8'?>

<dolfin xmlns:dolfin='http://www.fenics.org/dolfin/'>
  <parameters>
    <parameter name='tolerance' type='real' value='0.01'/>
    <parameter name='number of samples' type='int' value='10'/>
    <parameter name='solve dual problem' type='bool' value='false'/>
    <parameter name='file name' type='string' value='solution.xml'/>
  </parameters>
</dolfin>
```

Chapter 11

Solvers

DOLFIN provides a number of pre-defined PDE solvers (called “modules” in the source structure) by default. The solver interface is intentionally very simple to facilitate users writing their own solvers. These are the pre-defined solvers:

1. Poisson
2. Convection-Diffusion
3. Navies-Stokes
4. Elasticity

A solver for a PDE should provide the following interface:

1. a constructor which takes a mesh, equation coefficients and possibly additional data.
2. a `solve()` method which solves the equation given the specified data.
3. a static `solve()` function which constructs and solves the equation.

FIXME: List solvers, then present in detail, include lots of nice images with solver output

11.1 Poisson's equation

Poisson's equation with Dirichlet and homogenous Neumann boundary conditions:

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= g_D && \text{on } \Gamma_1, \\ -\partial_n u &= 0 && \text{on } \Gamma_2 \end{aligned} \tag{11.1}$$

The variational formulation is given by

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v. \tag{11.2}$$

The boundary conditions are enforced strongly and thus don't appear in the variational formulation.

11.1.1 Usage

The API for the Poisson solver:

```
// Create Poisson solver
PoissonSolver(Mesh& mesh, Function& f, BoundaryCondition& bc);

// Solve Poisson's equation
void solve();

// Solve Poisson's equation (static version)
static void solve(Mesh& mesh, Function& f, BoundaryCondition& bc);
```


A simple example of using the solver:

```
int main()
{
    Mesh mesh("mesh.xml.gz");
    MyFunction f;
    MyBC bc;

    PoissonSolver::solve(mesh, f, bc);

    return 0;
}
```

Where “f” is a Function specifying the right-hand side of the equation and “bc” is a BoundaryCondition.

11.1.2 Performance

The solver is an illustrative example and performance has not been a goal. It uses a GMRES linear solver, where a multi-grid linear solver would give optimal performance.

11.1.3 Limitations

The solver is meant to be the simplest example solver, and therefore some simplifications have been made. Typically the general form of Poisson’s equation includes a diffusion coefficient which has been omitted here.

11.2 Convection–diffusion

The convection-diffusion equation with Dirichlet and homogenous Neumann boundary conditions is given by:

$$\begin{aligned}
\dot{u} + b \cdot \nabla u - \nabla \cdot (a \nabla u) &= f \quad \text{in } \Omega \times (0, T], \\
u &= g_D \quad \text{on } \Gamma_1 \times (0, T], \\
-\partial_n u &= 0 \quad \text{on } \Gamma_2 \times (0, T], \\
u(\cdot, 0) &= u_0 \quad \text{in } \Omega,
\end{aligned} \tag{11.3}$$

where the convection is given by the vector $b = b(x, t)$ and the diffusion is given by $a = a(x, t)$.

The variational formulation is:

FIXME:Stabilized convection-diffusion

This is a stabilized FEM-formulation, so the solver can handle convection-dominated problems.

The time integration is done using cG(1) (Crank-Nicolson).

11.2.1 Usage

The API for the convection-diffusion solver:

```

// Create convection-diffusion solver
ConvectionDiffusionSolver(Mesh& mesh, Function& w, Function& f,
    BoundaryCondition& bc);

// Solve convection-diffusion
void solve();

// Solve convection-diffusion (static version)
static void solve(Mesh& mesh, Function& w, Function& f,
    BoundaryCondition& bc);

```

A simple example of using the solver:

```
int main()
{
    dolfin_output("curses");

    Mesh mesh("dolfin.xml.gz");
    Convection w;
    Source f;
    MyBC bc;

    ConvectionDiffusionSolver::solve(mesh, w, f, bc);

    return 0;
}
```

11.2.2 Performance

There are no particular performance issues with the solver. GMRES is used for solving the linear system.

11.2.3 Limitations

Currently many coefficients (such as diffusivity) are not user-definable, they need to be exposed by the interface.

11.3 Incompressible Navier–Stokes

Write introduction here, equations etc.

11.3.1 Usage

Present API of solver and give an example.

11.3.2 Performance

Write something about the performance of the solver.

11.3.3 Limitations

Write something about the limitations of the solver.

11.4 Elasticity

Navier's equations of elasticity with Dirichlet and homogenous Neumann boundary conditions:

$$\begin{aligned}
 u &= x - X, \\
 \dot{u} - v &= 0 \quad \text{in } \Omega^0, \\
 \dot{v} - \nabla \cdot \sigma &= f \quad \text{in } \Omega^0, \\
 \sigma &= E\epsilon(u) = E(\nabla u^\top + \nabla u) \\
 E\epsilon &= \lambda \text{tr}(\epsilon)I + 2\mu\epsilon, \\
 v(0, \cdot) &= v^0, \quad u(0, \cdot) = u^0 \quad \text{in } \Omega^0, \\
 u &= g_D \quad \text{on } \Gamma_1 \times (0, T], \\
 -\partial_n u &= 0 \quad \text{on } \Gamma_2 \times (0, T]
 \end{aligned}$$

The variational form:

$$\int_{\Omega} \dot{v}w \, dx = \int_{\Omega} -\sigma(u)\epsilon(v) + fw \, dx, \quad \forall w. \quad (11.4)$$

The time integration is done using dG(0) (backward Euler).

The mass matrix appearing from $\int_{\Omega} \dot{v}w \, dx$ is lumped (equivalent to computing it using nodal quadrature).

11.4.1 Usage

Present API of solver and give an example.

11.4.2 Performance

Write something about the performance of the solver.

11.4.3 Limitations

Write something about the limitations of the solver.

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Appendix A

Reference elements

A.1 The reference triangle

The reference triangle (Figure A.1) is defined by the following three vertices:

$$\begin{aligned}v^0 &= (0, 0), \\v^1 &= (1, 0), \\v^2 &= (0, 1).\end{aligned}\tag{A.1}$$

Note that this corresponds to a counter-clockwise orientation of the vertices in the plane.

The edges of the reference triangle are ordered following the convention that edge e^i should be opposite to vertex v^i for $i = 0, 1, 2$, with the vertices of each edge ordered to give a counter-clockwise orientation of the triangle in the plane:

$$\begin{aligned}e^0 &: (v^1, v^2), \\e^1 &: (v^2, v^0), \\e^2 &: (v^0, v^1).\end{aligned}\tag{A.2}$$

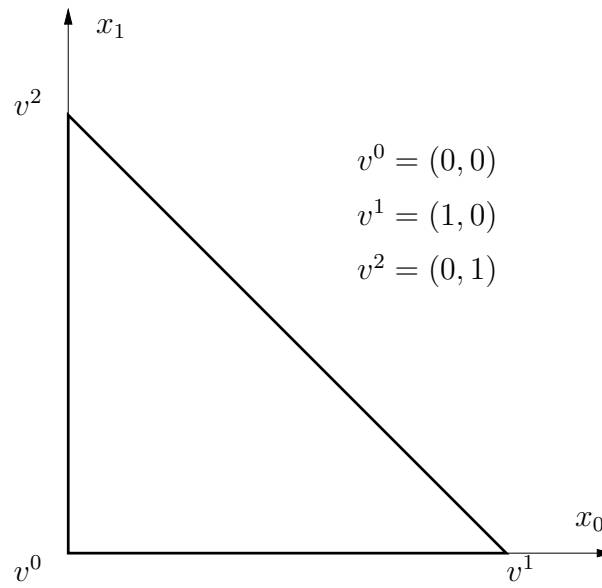


Figure A.1: Physical coordinates of the reference triangle.

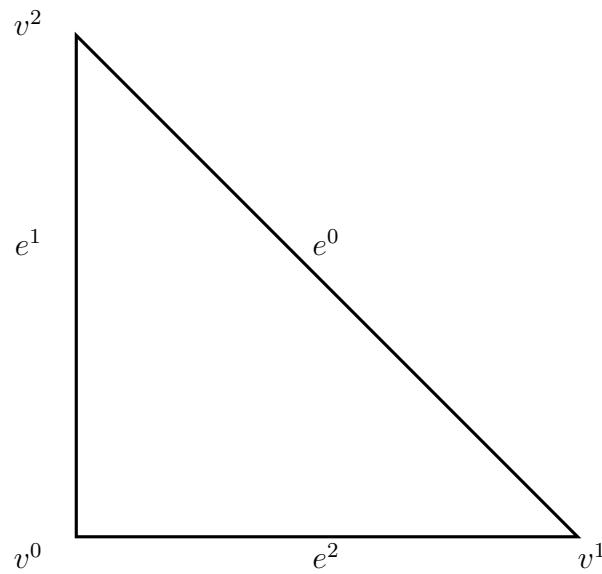


Figure A.2: Ordering of mesh entities (vertices and edges) for the reference triangle.

A.2 The reference tetrahedron

The reference tetrahedron (Figure A.3) is defined by the following four vertices:

$$\begin{aligned} v^0 &= (0, 0, 0), \\ v^1 &= (1, 0, 0), \\ v^2 &= (0, 1, 0), \\ v^3 &= (0, 0, 1). \end{aligned} \tag{A.3}$$

The faces of the reference tetrahedron are ordered following the convention that face f^i should be opposite to vertex v^i for $i = 0, 1, 2, 3$, with the vertices of each face ordered to give a counter-clockwise orientation of each face as seen from the outside of the tetrahedron and the first vertex of face f^i given by vertex $v^{i+1 \bmod 4}$:

$$\begin{aligned} f^0 &: (v^1, v^3, v^2), \\ f^1 &: (v^2, v^3, v^0), \\ f^2 &: (v^3, v^1, v^0), \\ f^3 &: (v^0, v^1, v^2). \end{aligned} \tag{A.4}$$

The edges of the reference tetrahedron are ordered following the convention that edges e^0, e^1, e^2 should correspond to the edges of the reference triangle. Edges e^3, e^4, e^5 all ending up at vertex v^3 are ordered based on their first vertex:

$$\begin{aligned} e^0 &: (v^1, v^2), \\ e^1 &: (v^2, v^0), \\ e^2 &: (v^0, v^1), \\ e^3 &: (v^0, v^3), \\ e^4 &: (v^1, v^3), \\ e^5 &: (v^2, v^3). \end{aligned} \tag{A.5}$$

The ordering of vertices on faces implicitly defines an ordering of edges on

faces by identifying an edge on a face with the opposite vertex on the face:

$$\begin{aligned}
 f^0 &: (e^5, e^0, e^4), \\
 f^1 &: (e^3, e^1, e^5), \\
 f^2 &: (e^2, e^3, e^4), \\
 f^3 &: (e^0, e^1, e^2).
 \end{aligned}
 \tag{A.6}$$

Note that the ordering of edges on f^3 is the same as the ordering of edges on the reference triangle. Also note that the internal ordering of vertices on edges does not always follow the orientation of the face (which is not possible).

A.3 Ordering of degrees of freedom

The local and global orderings of degrees of freedom or *nodes* are obtained by associating each node with a mesh entity, locally and globally.

A.3.1 Mesh entities

We distinguish between mesh entities of different topological dimensions:

<i>vertices</i>	topological dimension 0
<i>edges</i>	topological dimension 1
<i>faces</i>	topological dimension 2
<i>cells</i>	topological dimension 2 or 3

A cell can be either a triangle or a tetrahedron depending on the type of mesh. For a mesh consisting of triangles, the mesh entities involved are vertices, edges and cells, and for a mesh consisting of tetrahedrons, the mesh entities involved are vertices, edges, faces and cells.

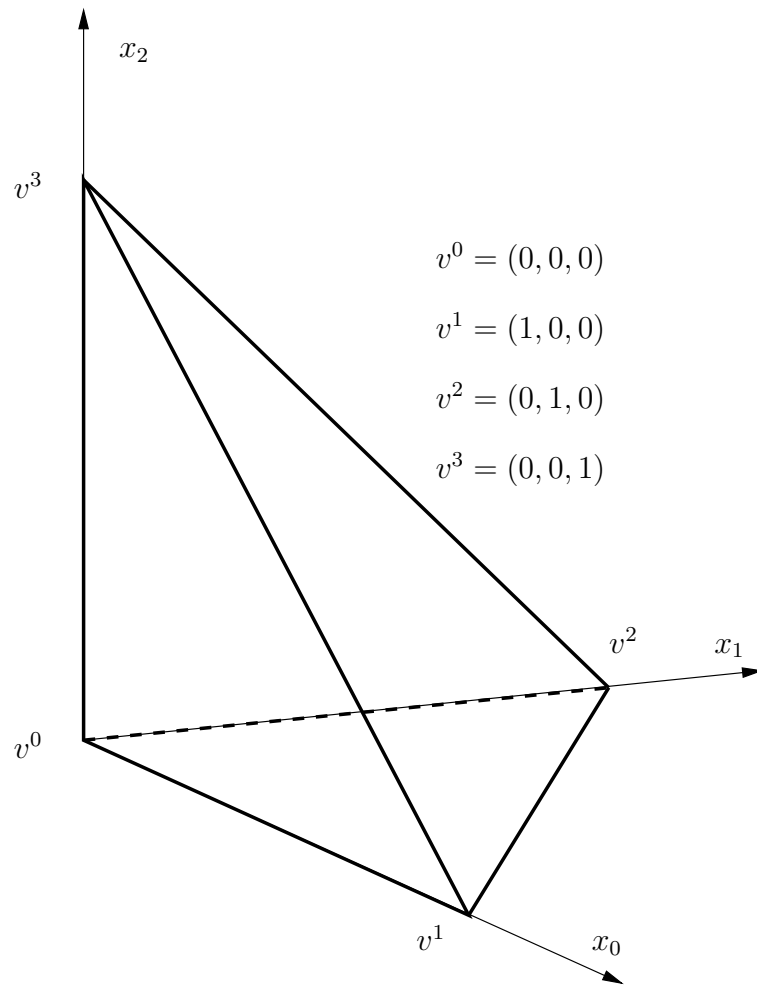


Figure A.3: Physical coordinates of the reference tetrahedron.

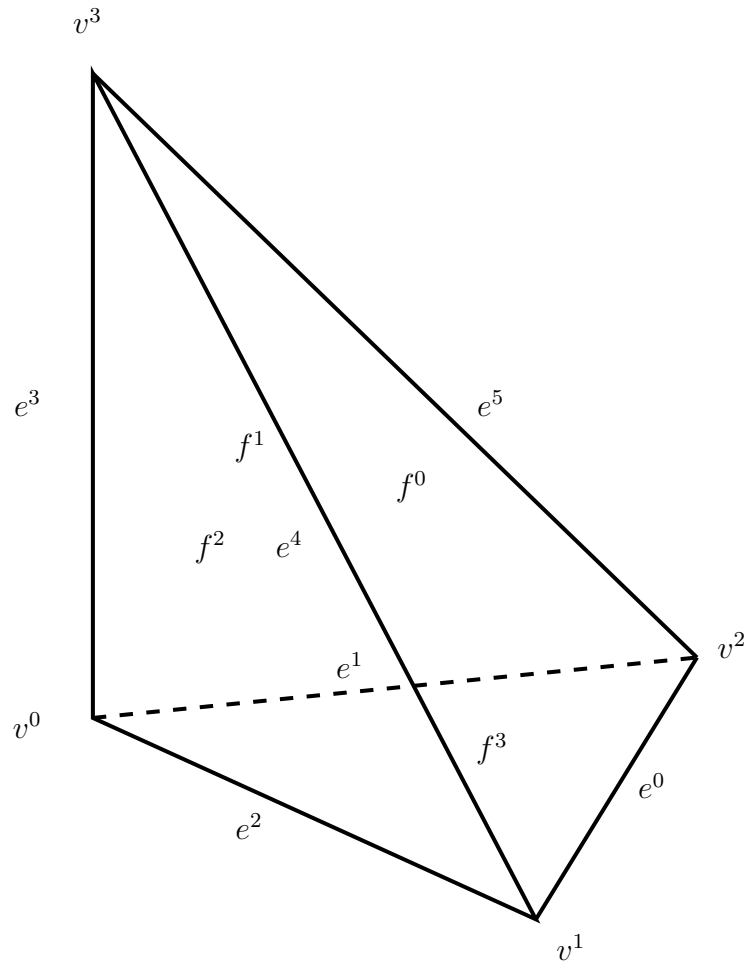


Figure A.4: Ordering of mesh entities (vertices, edges, faces) for the reference tetrahedron.

A.3.2 Ordering among mesh entities

With each mesh entity, there can be associated zero or more nodes and the nodes are ordered locally and globally based on the topological dimension of the mesh entity with which they are associated. Thus, any nodes associated with vertices are ordered first and nodes associated with cells last.

If more than one node is associated with a single mesh entity, the internal ordering of the nodes associated with the mesh entity becomes important, in particular for edges and faces, where the nodes of two adjacent cells sharing a common edge or face must line up.

A.3.3 Internal ordering on edges

For edges containing more than one node, the nodes are ordered in the direction from the first vertex (v_e^0) of the edge to the second vertex (v_e^1) of the edge as in Figure A.5.

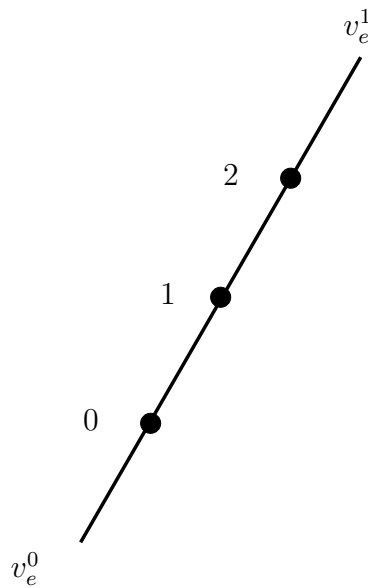


Figure A.5: Internal ordering of nodes on edges.

A.3.4 Alignment of edges

Depending on the orientation of any given cell, an edge on the cell may be aligned or not aligned with the corresponding edge on the reference cell if the vertices of the cell are mapped to the reference cell. We define the *alignment* of an edge with respect to a cell to be 0 if the edge is aligned with the orientation of the reference cell and 1 otherwise.

Example 1: The alignment of the first edge (e^0) on a triangle is 0 if the first vertex of the edge is the second vertex (v^1) of the triangle.

Example 2: The alignment of the second edge (e^1) on a tetrahedron is 0 if the first vertex of the edge is the third vertex (v^2) of the tetrahedron.

If two cells share a common edge and the edge is aligned with one of the cells and not the other, we must reverse the order in which the local nodes are mapped to global nodes on one of the two cells. As a convention, the order is kept if the alignment is 0 and reversed if the alignment is 1.

A.3.5 Internal ordering on faces

For faces containing more than one node, the ordering of nodes is nested going from the first to the third vertex and in each step going from the first to the second vertex as in Figure A.6.

A.3.6 Alignment of faces

There are six different ways for a face to be aligned on a tetrahedron; there are three ways to pick the first edge of the face, and once the first edge is picked, there are two ways to pick the second edge. To define an alignment of faces as an integer between 0 and 5, we compare the ordering of edges on a face with the ordering of edges on the corresponding face on the reference tetrahedron. If the first edge of the face matches the first edge on the corresponding face on the reference tetrahedron and also the second edge matches the second edge on the reference tetrahedron, then the alignment is 0. If only the first

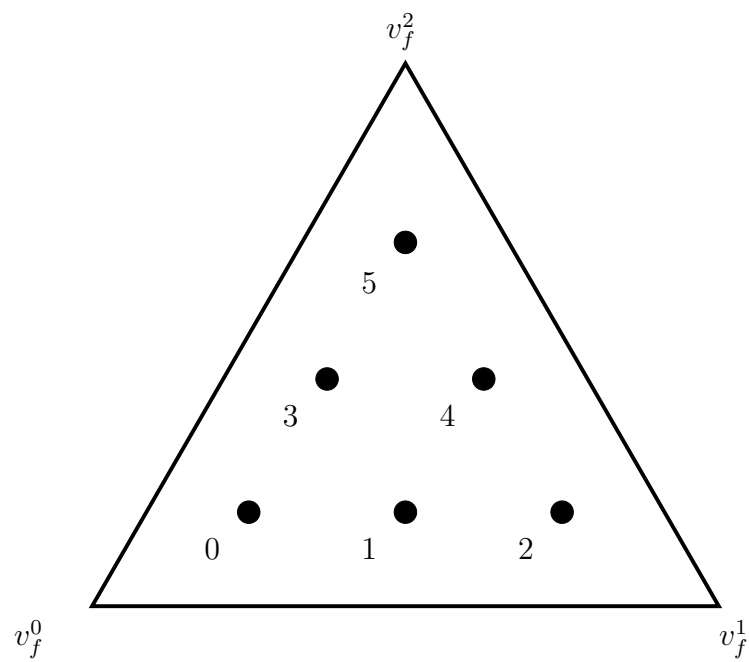


Figure A.6: Internal ordering of nodes on faces.

edge matches, then the alignment is 1. We similarly define alignments 2, 3 by matching the first and second edges with the second and third edges on the corresponding face on the reference tetrahedron, and alignments 4, 5 by matching the first and second edges with the third and first edges on the corresponding face on the reference tetrahedron.

Example 1: The alignment of the first face of a tetrahedron is 0 if the first edge of the face is edge number 5 and the second edge is edge number 0.

Example 2: The alignment of the first face of a tetrahedron is 1 if the first edge of the face is edge number 5 and the second edge is not edge number 0. (It must then be edge number 4.)

Example 3: The alignment of the first face of a tetrahedron is 4 if the first edge of the face is edge number 4 and the second edge is edge number 5.

Example 4: The alignment of the first face of a tetrahedron is 5 if the first edge of the face is edge number 4 and the second edge is not edge number 5. (It must then be edge number 0.)

Appendix B

Installation

The source code of **DOLFIN** is portable and should compile on any Unix system, although it is developed mainly under GNU/Linux (in particular Debian GNU/Linux). **DOLFIN** can be compiled under Windows through Cygwin [1]. Questions, bug reports and patches concerning the installation should be directed to the **DOLFIN** mailing list at the address

`dolfin-dev@fenics.org`

DOLFIN must currently be compiled directly from source, but effort is underway to provide precompiled Debian packages of **DOLFIN** and other **FENICS** components.

B.1 Installing from source

B.1.1 Dependencies and requirements

DOLFIN depends on a number of libraries that need to be installed on your system. These libraries include Libxml2 and PETSc. In addition to these

libraries, you need to install **FIAT** and **FFC** if you want to define your own variational forms.

Installing Libxml2

Libxml2 is a library used by **DOLFIN** to parse XML data files. Libxml2 can be obtained from

<http://xmlsoft.org/>

Packages are available for most Linux distributions. For Debian users, the package to install is `libxml2-dev`.

Installing PETSc

PETSc is a library for the solution of linear and nonlinear systems, functioning as the backend for the **DOLFIN** linear algebra classes. **DOLFIN** depends on PETSc version 2.3.0, which can be obtained from

<http://www-unix.mcs.anl.gov/petsc/petsc-2/>

Follow the installation instructions on the PETSc web page. Normally, you should only have to perform the following simple steps in the PETSc source directory:

```
# export PETSC_DIR='pwd'
# ./config/configure.py --with-clanguage=cxx --with-shared=1
# make all
```

Add `--download-hypre=yes` to `configure.py` if you want to install Hypre which provides a collection of preconditioners, including algebraic multigrid (AMG).

DOLFIN assumes that `PETSC_DIR` is `/usr/local/lib/petsc/` but this can be controlled using the flag `--with-petsc-dir=<path>` when configuring DOLFIN (see below).

Installing FFC

DOLFIN uses the FEniCS Form Compiler **FFC** to process variational forms. **FFC** can be obtained from

<http://www.fenics.org/>

Follow the installation instructions given in the **FFC** manual. **FFC** follows the standard for Python packages, which means that normally you should only have to perform the following simple step in the **FFC** source directory:

```
# python setup.py install
```

Note that **FFC** depends on **FIAT**, which in turn depends on the Python packages Numeric (Debian package `python-numeric`) and LinearAlgebra (Debian package `python-numeric-ext`). Refer to the **FFC** manual for further details.

B.1.2 Downloading the source code

The latest release of **DOLFIN** can be obtained as a `tar.gz` archive in the download section at

<http://www.fenics.org/>

Download the latest release of **DOLFIN**, for example `dolfin-0.1.0.tar.gz`, and unpack using the command

```
# tar xzfv dolfin-0.1.0.tar.gz
```

This creates a directory `dolfin-0.1.0` containing the **DOLFIN** source code.

If you want the very latest version of **DOLFIN**, there is also a version named `dolfin-cvs-current.tar.gz` which provides a snapshot of the current CVS version of **DOLFIN**, updated automatically from the CVS repository each hour. This version may contain features not yet present in the latest release, but may also be less stable and even not work at all.

B.1.3 Compiling the source code

DOLFIN is built using the standard GNU Autotools (Automake, Autoconf), which means that the installation procedure is simple:

```
# ./configure
# make
```

followed by an optional

```
# make install
```

to install **DOLFIN** on your system.

The configure script will check for a number of libraries and try to figure out how compile **DOLFIN** against these libraries. The configure script accepts a collection of optional arguments that can be used to control the compilation process. A few of these are listed below. Use the command

```
# ./configure --help
```

for a complete list of arguments.

- Use the option `--prefix=<path>` to specify an alternative directory for installation of **DOLFIN**. The default directory is `/usr/local/`, which

means that header files will be installed under `/usr/local/include/` and libraries will be installed under `/usr/local/lib/`. This option can be useful if you don't have root access but want to install **DOLFIN** locally on a user account as follows:

```
# mkdir ~/local
# ./configure --prefix=~/local
# make
# make install
```

- Use the option `--enable-debug` to compile **DOLFIN** with debugging symbols and assertions.
- Use the option `--enable-optimization` to compile an optimized version of **DOLFIN** without debugging symbols and assertions.
- Use the option `--disable-curses` to compile **DOLFIN** without the curses interface (a text-mode graphical user interface).
- Use the option `--disable-mpi` to compile **DOLFIN** without support for MPI (Message Passing Interface), assuming PETSc has been compiled without support for MPI.
- Use the option `--with-petsc-dir=<path>` to specify the location of the PETSc directory. By default, **DOLFIN** assumes that PETSc has been installed in `/usr/local/lib/petsc/`.

B.1.4 Compiling the demo programs

After compiling the **DOLFIN** library according to the instructions above, you may want to try one of the demo programs in the subdirectory `src/demo/` of the **DOLFIN** source tree. Just enter the directory containing the demo program you want to compile and type `make`. You may also compile all demo programs at once using the command

```
# make demo
```

B.1.5 Compiling a program against DOLFIN

Whether you are writing your own Makefiles or using an automated build system such as GNU Autotools or BuildSystem, it is straightforward to compile a program against **DOLFIN**. The necessary include and library paths can be obtained through the script `dolfin-config` which is automatically generated during the compilation of **DOLFIN** and installed in the `bin` subdirectory of the `<path>` specified with `--prefix`. Assuming this directory is in your executable path (environment variable `PATH`), the include path for building **DOLFIN** can be obtained from the command

```
dolfin-config --cflags
```

and the path to **DOLFIN** libraries can be obtained from the command

```
dolfin-config --libs
```

If `dolfin-config` is not in your executable path, you need to provide the full path to `dolfin-config`.

Examples of how to write a proper `Makefile` are provided with each of the example programs in the subdirectory `src/demo/` in the **DOLFIN** source tree.

B.2 Debian package

In preparation.

B.3 Installing from source under Windows

DOLFIN can be used under Windows using Cygwin, which provides a Linux-like environment. The installation process is largely the same as under GNU/Linux. This section addresses some Cygwin specific issues.

To use **DOLFIN** under Cygwin, the Cygwin development tools must be installed. Instructions for installing PETSc under Cygwin can be found on the PETSc web page. Installation of **FFC** and **FIAT** is the same as under GNU/Linux. The Python package Numeric is not available as a Cygwin package and must be installed manually. To compile **DOLFIN**, the Cygwin package `libxml2-devel` must be installed. **DOLFIN** does not link correctly with the curses libraries of Cygwin, so under Cygwin, **DOLFIN** can be built by:

```
# ./configure --disable-curses
# make
```

If MPI has not been installed:

```
# ./configure --disable-mpi --disable-curses
# make
```

Due to problems with the latest GCC compilers provided by Cygwin (GCC 3.4.4), compiling **DOLFIN** will lead to fatal errors. These problems can be avoided by using GCC version 3.3.3 provided by Cygwin.

Appendix C

Contributing code

If you have created a new module, fixed a bug somewhere, or have made a small change which you want to contribute to **DOLFIN**, then the best way to do so is to send us your contribution in the form of a patch. A patch is a file which describes how to transform a file or directory structure into another. The patch is built by comparing a version which both parties have against the modified version which only you have.

C.1 Creating a patch

The tool used to create a patch is called `diff` and the tool used to apply the patch is called `patch`. These tools are free software and are standard on most Unix systems.

Here's an example of how it works. Start from the latest release of **DOLFIN**, which we here assume is release 0.1.0. You then have a directory structure under `dolfin-0.1.0` where you have made modifications to some files which you think could be useful to other users.

1. Clean up your modified directory structure to remove temporary and binary files which will be rebuilt anyway:

```
# make clean
```

2. From the parent directory, rename the **DOLFIN** directory to something else:

```
# mv dolfin-0.1.0 dolfin-0.1.0-mod
```

3. Unpack the version of **DOLFIN** that you started from:

```
# tar xzfv dolfin-0.1.0.tar.gz
```

4. You should now have two **DOLFIN** directory structures in your current directory:

```
# ls
dolfin-0.1.0
dolfin-0.1.0-mod
```

5. Now use the `diff` tool to create the patch:

```
# diff -u --new-file --recursive dolfin-0.1.0
dolfin-0.1.0-mod > dolfin-<identifier>-<date>.patch
```

written as one line, where `<identifier>` is a keyword that can be used to identify the patch as coming from you (your username, last name, first name, a nickname etc) and `<date>` is today's date in the format `yyyy-mm-dd`.

6. The patch now exists as `dolfin-<identifier>-<date>.patch` and can be distributed to other people who already have `dolfin-0.1.0` to easily create your modified version. If the patch is large, compressing it with for example `gzip` is advisable:

```
# gzip dolfin-<identifier>-<date>.patch
```

C.2 Sending patches

Patch files should be sent to the **DOLFIN** mailing list at the address

dolfin-dev@fenics.org

Include a short description of what your patch accomplishes. Small patches have a better chance of being accepted, so if you are making a major contribution, please consider breaking your changes up into several small self-contained patches if possible.

C.3 Applying a patch (maintainers)

Let's say that a patch has been built relative to **DOLFIN** release 0.1.0. The following description then shows how to apply the patch to a clean version of release 0.1.0.

1. Unpack the version of **DOLFIN** which the patch is built relative to:

```
# tar xzfv dolfin-0.1.0.tar.gz
```

2. Check that you have the patch `dolfin-<identifier>-<date>.patch` and the **DOLFIN** directory structure in the current directory:

```
# ls
dolfin-0.1.0
dolfin-<identifier>-<date>.patch
```

Unpack the patch file using `gunzip` if necessary.

3. Enter the **DOLFIN** directory structure:

```
# cd dolfin-0.1.0
```

4. Apply the patch:

```
# patch -p1 < ../dolfin-<identifier>-<date>.patch
```

The option `-p1` strips the leading directory from the filename references in the patch, to match the fact that we are applying the patch from inside the directory. Another useful option to `patch` is `--dry-run` which can be used to test the patch without actually applying it.

5. The modified version now exists as `dolfin-0.1.0`.

C.4 License agreement

By contributing a patch to **DOLFIN**, you agree to license your contributed code under the GNU General Public License (a condition also built into the GPL license of the code you have modified). Before creating the patch, please update the author and date information of the file(s) you have modified according to the following example:

```
// Copyright (C) 2004-2005 Johan Hoffman and Anders Logg.  
// Licensed under the GNU GPL Version 2.  
//  
// Modified by Johan Jansson 2005.  
// Modified by Garth N. Wells 2005.  
//  
// First added: 2004-06-22  
// Last changed: 2005-09-01
```

As a rule of thumb, the original author of a file holds the copyright.

Appendix D

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Version 2, June 1991

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