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# About this manual

This manual is currently being written. As a consequence, some sections may be incomplete or inaccurate. In particular, only the C++ interface (not the Python interface) of **DOLFIN** is documented, and only to a certain extent. Care has been taken that the quickstart chapter is accurate, but other than that, inconsistencies and inaccuracies can be expected.

We apologize for any inconvenience, but take comfort in the fact that (i) with the release of **DOLFIN** 0.7.0, the interface is starting to mature and will undergo less dramatic changes in the future (which will actually make it possible to write documentation) and (ii) most of the code is pretty well documented through the demos. If you have some writing skills and are willing to contribute, please consider writing a section or two and submit to the mailing list!

## 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

# 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 D for detailed installation instructions and Chapter 6 for a detailed discussion of how to solve partial differential equations with **DOLFIN**.

# 1.1 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 x.y.z of **DOLFIN**:

```
# tar zxfv dolfin-x.y.z.tar.gz
```

```
# cd dolfin-x.y.z
```

# sudo scons install

Since **DOLFIN** depends on a number of other packages, you may also need to download and install those packages before you can compile **DOLFIN**. (See Appendix **D** for detailed instructions.)

## 1.2 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  $\Gamma = \{(x,y) \in \partial\Omega : x = 0 \text{ or } x = 1\}$ , homogeneous Neumann boundary conditions  $\partial_n u = 0$  on the remaining part of the boundary, and right-hand side given by  $f(x,y) = 500 \exp(-((x-0.5)^2 + (y-0.5)^2)/0.02)$ :

$$-\Delta u(x,y) = f(x,y), \quad x \in \Omega = (0,1) \times (0,1), \tag{1.1}$$

$$u(x,y) = 0, \quad (x,y) \in \Gamma = \{(x,y) \in \partial\Omega : x = 0 \text{ or } x = 1\}, (1.2)$$

$$\partial_n u(x,y) = 0, \quad (x,y) \in \partial\Omega \setminus \Gamma.$$
 (1.3)

To solve a partial differential equation with **DOLFIN**, it must first be written in *variational form*. The (discrete) variational formulation of Poisson's equation reads: Find  $u_h \in V_h$  such that

$$a(v, u_h) = L(v) \quad \forall v \in \hat{V}_h, \tag{1.4}$$

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

$$a(v, u_h) = \int_{\Omega} \nabla v \cdot \nabla u_h \,\mathrm{d}x \tag{1.5}$$

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

$$L(v) = \int_{\Omega} v f \, \mathrm{d}x. \tag{1.6}$$

## 1.2.1 Setting up the variational formulation

The variational formulation (1.4) must be given to **DOLFIN** as a pair of bilinear and linear forms (a, L) using a form compiler like **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 = TestFunction(element)
u = TrialFunction(element)
f = Function(element)
a = dot(grad(v), grad(u))*dx
L = v*f*dx
```

The example is given here 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 -l dolfin Poisson.form

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

### 1.2.2 Writing the solver

Having compiled the variational formulation (1.4) 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 demo/pde/poisson/cpp/ of the **DOLFIN** source tree.<sup>1</sup>

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 in 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;
```

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:

```
// Include headers and define classes here
int main()
{
    // Write your program here
    return 0;
}
```

We now proceed to specify the right-hand side f of (1.1). This is done by defining a new subclass of Function (which we here name Source) and by overloading the eval() function to return the value  $f(x, y) = 500 \exp(-((x - 0.5)^2 + (y - 0.5)^2)/0.02)$ :

class Source : public Function
{

<sup>1</sup>A corresponding Python demo is available in demo/pde/poisson/python/

```
void eval(double* values, const double* x) const
{
    double dx = x[0] - 0.5;
    double dy = x[1] - 0.5;
    values[0] = 500.0*exp(-(dx*dx + dy*dy) / 0.02);
};
```

To define the Dirichlet boundary condition, we define a SubDomain for the Dirichlet boundary:

```
class DirichletBoundary : public SubDomain
{
    bool inside(const double* x, bool on_boundary) const
    {
       return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EPS;
    }
};
```

Next, we need to create a mesh. **DOLFIN** relies on external programs for mesh generation, and imports meshes in **DOLFIN** XML format. Meshes in other formats can be converted to the **DOLFIN** XML format using the script dolfin-convert. 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 1/32 (with a total of  $2 \cdot 32^2 = 2048$  triangles), we can just type

UnitSquare mesh(32, 32);

Next, we instantiate a finite element function space on the mesh as follows:

PoissonFunctionSpace V(mesh);

Here, we make use of the code generated by the form compiler (the class PoissonFunctionSpace).

Next, we define the Dirichlet boundary condition by specifying the value that the solution should take and the subset of the boundary where it should be applied:

Constant u0(0.0); DirichletBoundary boundary; DirichletBC bc(V, u0, boundary);

Note the difference in how Dirichlet and Neumann boundary conditions are applied. Dirichlet conditions are here applied strongly (but may also be applied weakly) using the DirichletBC class, while Neumann boundary conditions are defined as part of the variational problem. (It is a *natural* boundary condition for this variational formulation of Poisson's equation.)

Next, we initialize the pair of bilinear and linear forms that we have previously compiled with **FFC**. We also instantiate the right-hand side function and attach it to the linear form:

```
PoissonBilinearForm a(V, V);
PoissonLinearForm L(V);
Source f;
L.f = f;
```

To solve the variational problem, we use the class VariationalProblem, which automatically assembles and solves the corresponding linear system:

```
VariationalProblem problem(a, L, bc);
Function u;
problem.solve(u);
```

To plot the solution, one may simply type

plot(u);

This requires the installation of PyDOLFIN and Viper. (A warning will be issued if plotting is not available.)

Finally, we export the solution **u** to a file for visualization. Here, we choose to save the solution in VTK format for visualization in ParaView or MayaVi, which we do by specifying a file name with extension .pvd:

```
File file("poisson.pvd");
file << u;</pre>
```

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

```
#include <dolfin.h>
#include "Poisson.h"
using namespace dolfin;
// Source term
class Source : public Function
{
  void eval(double* values, const double* x) const
  ſ
    double dx = x[0] - 0.5;
    double dy = x[1] - 0.5;
    values[0] = 500.0*exp(-(dx*dx + dy*dy) / 0.02);
 }
};
// Sub domain for Dirichlet boundary condition
class DirichletBoundary : public SubDomain
{
 bool inside(const double* x, bool on_boundary) const
  {
```

```
return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EPS;
  }
};
int main()
{
  // Create mesh and function space
  UnitSquare mesh(32, 32);
  PoissonFunctionSpace V(mesh);
  // Define boundary condition
  Constant u0(0.0);
  DirichletBoundary boundary;
  DirichletBC bc(V, u0, boundary);
  // Define variational problem
  PoissonBilinearForm a(V, V);
  PoissonLinearForm L(V);
  Source f;
  L.f = f;
  // Compute solution
  VariationalProblem problem(a, L, bc);
  Function u;
  problem.solve(u);
  // Plot solution
  plot(u);
  // Save solution in VTK format
  File file("poisson.pvd");
  file << u;</pre>
  return 0;
}
```

### 1.2.3 Compiling the program

The easiest way to compile the program is to create a SConstruct file that tells scons how to build the program. The following example shows how to write a SConstruct file for the above example:

```
import os, commands
# Get compiler from pkg-config
compiler = commands.getoutput('pkg-config --variable=compiler dolfin')
# Create a SCons Environment based on the main os environment
env = Environment(ENV=os.environ, CXX=compiler)
# Get compiler flags from pkg-config
env.ParseConfig('pkg-config --cflags --libs dolfin')
# Program name
env.Program('demo', 'main.cpp')
```

With this file in place, we just need to type scons to compile the program, generating the executable as the file demo. Note that this requires pkg-config to be able to find the file dolfin.pc. That file is generated by the configure script during the configuration of **DOLFIN**. If pkg-config fails to find it, you need to add the directory containing it to the environment variable PKG\_CONFIG\_PATH.

#### 1.2.4 Running the program

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

# ./demo

## 1.2.5 Visualizing the solution

The solution may be visualized either by the built-in plot() command or by calling an external application. The built-in plotting requires the installation of both PyDOLFIN and Viper. In this example, we chose to save the solution in VTK format, which can be imported into for example ParaView or MayaVi.

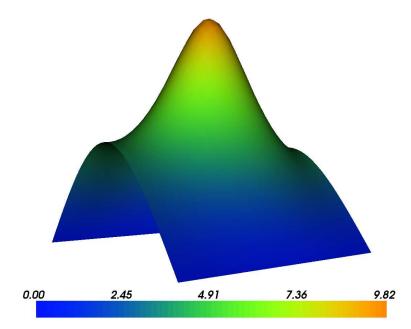


Figure 1.1: The solution of Poisson's equation (1.1) visualized using the plot() command (Viper).

# Chapter 2

# Linear algebra

► Developer's note: Since this chapter was written, the **DOLFIN** linear algebra interface has undergone some changes that are not documented here. As a result, some of the information in this chapter may be outdated, incomplete or simply wrong.

**DOLFIN** provides a high-performance linear algebra library, including matrices and vectors, a set of linear solvers, preconditioners, and an eigenvalue solver. The core part of the functionality is provided through wrappers that provide a common interface to the functionality of the linear algebra libraries uBLAS [13], PETSc [8] and Trilinos [?].

# 2.1 Matrices and vectors

The two basic linear algebra data structures are the classes Matrix and Vector, representing a sparse  $M \times N$  matrix and a vector of length N respectively.

The following code demonstrates how to create a matrix and a vector:

Matrix A(M, N);

Vector x(N);

Alternatively, the matrix and the vector may be created by

Matrix A; Vector x; A.init(M, N); x.init(N);

The following code demonstrates how to access the size and the elements of a matrix and a vector:

```
A(5, 5) = 1.0;
double a = A(4, 3);
x(3) = 2.0;
double b = x(5);
unsigned int M = A.size(0);
unsigned int N = A.size(1);
N = x.size();
```

In addition, **DOLFIN** provides optimized functions for setting the values of a set of entries in a matrix or vector:

```
double block[] = {2, 4, 6};
int rows[] = {0, 1, 2};
int cols[] = {0, 1, 2};
A.set(block, rows, cols, 3);
```

Alternatively, the set of values given by the array **block** can be added to the entries given by the arrays **rows** and **cols**:

```
double block[] = {2, 4, 6};
int rows[] = {0, 1, 2};
int cols[] = {0, 1, 2};
A.add(block, rows, cols, 3);
```

These functions are particularly useful for efficient assembly of a (sparse) matrix from a bilinear form.

### 2.1.1 Sparse matrices

The default **DOLFIN** class Matrix is a sparse matrix, which efficiently represents the discretization of a partial differential equation where most entries in the matrix are zero. Alternatively, the class SparseMatrix may be used which is identical with the class Matrix<sup>1</sup>.

If **DOLFIN** has been compiled with support for PETSc, then the sparse matrix is represented as a sparse PETSc matrix<sup>2</sup>. Alternatively, the class PETScMatrix may be used, together with the corresponding class PETScVector.

If **DOLFIN** has been compiled without support for PETSc, then the sparse matrix is represented as a uBLAS sparse matrix. Alternatively, the class uBLASSparseMatrix may be used, together with the corresponding class uBLASVector.

<sup>&</sup>lt;sup>1</sup>The class Matrix is a typedef for the class SparseMatrix.

 $<sup>^{2}</sup>$ By default, the sparse matrix is represented as a PETSc MATSEQAIJ matrix, but other PETSc representations are also available.

### 2.1.2 Dense matrices

**DOLFIN** provides the class **DenseMatrix** for representation of dense matrices. A dense matrix representation is often preferable when computing with matrices of small to moderate size. In particular, accessing individual elements is more efficient with a dense matrix representation.

A DenseMatrix is represented as uBLAS dense matrix and alternatively the class uBLASDenseMatrix may be used, together with the corresponding class uBLASVector.

### 2.1.3 The common interface

Although **DOLFIN** differentiates between sparse and dense data structures, the two classes GenericMatrix and GenericVector define a common interface to all matrices and vectors. Refer to the *DOLFIN programmer's* reference for the exact specification of these interfaces.

The following points should be noted:

- 1. If you want a specific backend like PETSc, then use PETScVector/PETScMatrix.
- 2. If you don't care about the backend, then use Vector/Matrix.
- 3. If you write a *function* that should be able to accept vectors and matrices from any backend as input, then use GenericVector/GenericMatrix.

## 2.2 Solving linear systems

**DOLFIN** provides a set of efficient solvers for linear systems of the form

$$Ax = b, (2.1)$$

where A is an  $N \times N$  matrix and where x and b are vectors of length N. Both iterative (Krylov subspace) solvers and direct (LU) solvers are provided.

### 2.2.1 Iterative methods

A linear system may be solved by the GMRES Krylov method as follows:

Matrix A; Vector x, b: GMRES::solve(A, x, b);

Alternatively, the linear system may be solved by first creating an object of the class KrylovSolver, which is more efficient for repeated solution of linear systems and also allows the specification of both the Krylov method and the preconditioner:

```
KrylovSolver solver(gmres, ilu);
solver.solve(A, x, b);
```

For uBLAS matrices and vectors, the class uBLASKrylovSolver may be used and for PETSc matrices and vectors, the class PETScKrylovSolver may be used.

#### Krylov methods

**DOLFIN** provides the following set of Krylov methods:

cg	The conjugate gradient method	
gmres	The GMRES method	
bicgstab	The stabilized biconjugate gradient squared method	
default_method	Default choice of Krylov method	

#### Preconditioners

**DOLFIN** provides the following set of preconditioners:

none	No preconditioning	
jacobi	Simple Jacobi preconditioning	
sor SOR, successive over-relaxation		
ilu Incomplete LU factorization		
icc	Incomplete Cholesky factorization	
amg Algebraic multigrid (through Hypre when av		
default_pc Default choice of preconditioner		

#### Matrix-free solvers

The **DOLFIN** Krylov solvers may be used without direct access to a matrix representation. All that is needed is to provide the size of the linear system, the right-hand side, and a method implementing the multiplication of the matrix with any given vector.

Such a "virtual matrix" may be defined by implementing the interface defined by either the class uBLASKrylovMatrix of PETScKrylovMatrix. The matrix may then be used together with either the class uBLASKrylovSolver or PETScKrylovSolver.

#### 2.2.2 Direct methods

A linear system may be solved by a direct LU factorization as follows:

```
Matrix A;
Vector x, b;
LU::solve(A, x, b);
```

Alternatively, the linear system may be solved by first creating an object of the class LUSolver, which may be more efficient for repeated solution of linear systems:

LUSolver solver; solver.solve(A, x, b);

For uBLAS matrices and vectors, the class uBLASLUSolver may be used and for PETSc matrices and vectors, the class PETScLUSolver may be used.

## 2.3 Eigenvalue problems

**DOLFIN** also provides a solver for eigenvalue problems. The solver is only available when **DOLFIN** has been compiled with support for PETSc and SLEPc [12].

For the basic eigenvalue problem

$$Ax = \lambda x, \tag{2.2}$$

the following code demonstrates how to compute the first eigenpair:

```
SLEPcEigenvalueSolver esolver;
esolver.solve(A);
double lr, lc;
PETScVector xr, xc;
esolver.getEigenpair(lr, lc, xr, xc, 0);
```

The double and complex components of the eigenvalue are returned in lr and lc, respectively, and the double and complex parts of the eigenvector are returned in xr and xc, respectively.

For the generalized eigenvalue problem

$$Ax = \lambda Bx, \tag{2.3}$$

the following code demonstrates how to compute the third eigenpair:

```
PETScEigenvalueSolver esolver;
esolver.solve(A, B);
double lr, lc;
PETScVector xr, xc;
esolver.getEigenpair(lr, lc, xr, xc, 2);
```

## 2.4 Linear algebra backends

#### 2.4.1 uBLAS

uBLAS is a C++ template library that provides BLAS level 1, 2 and 3 functionality (and more) for dense, packed and sparse matrices. The design and implementation unify mathematical notation via operator overloading and efficient code generation via expression templates.

**DOLFIN** wrappers for uBLAS linear algebra is provided through the classes uBLASSparseMatrix, uBLASDenseMatrix and uBLASVector. These classes are implemented by subclassing the corresponding uBLAS classes, which means that all standard uBLAS operations are supported for these classes. For advanced usage not covered by the common **DOLFIN** interface specified by the classes **GenericMatrix** and **GenericVector**, refer directly to the documentation of uBLAS.

#### 2.4.2 **PETSc**

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.

**DOLFIN** wrappers for PETSc linear algebra is provided through the classes PETScMatrix and PETScVector. Direct access to the PETSc data structures is available through the member functions mat() and vec(), which return the PETSc Mat and Vec pointers respectively. For advanced usage not covered by the common **DOLFIN** interface specified by the classes GenericMatrix and GenericVector, refer directly to the documentation of PETSc.

## 2.4.3 Trilinos

Trilinos . . . .

## 2.4.4 Matrix Template Library (MTL4)

MTL4 . . . .

## 2.4.5 User provided linear algebra backends

 $\blacktriangleright$  Developer's note: This section will explain how a user-provided linear alegra backend can be used with **DOLFIN**.

# Chapter 3

# The mesh

► Developer's note: This chapter is just a quick write-up of the most basic functionality of the mesh library and will be expanded.

## **3.1** Basic concepts

## 3.1.1 Mesh

A *mesh* consists of *mesh* topology and *mesh* geometry. These concepts are implemented by the classes Mesh, MeshTopology and MeshGeometry.

#### **3.1.2** Mesh entities

A mesh entity is a pair (d, i), where d is the topological dimension of the mesh entity and i is a unique index of the mesh entity. Mesh entities are numbered within each topological dimension from 0 to  $n_d - 1$ , where  $n_d$  is the number of mesh entities of topological dimension d.

For convenience, mesh entities of topological dimension 0 are referred to as

*vertices*, entities of dimension 1 *edges*, entities of dimension 2 *faces*, entities of *codimension* 1 *facets* and entities of codimension 0 *cells*. These concepts are summarized in Table 3.1.

Entity	Dimension	Codimension
Vertex	0	_
Edge	1	_
Face	2	_
Facet	—	1
Cell	_	0

Table 3.1: Named mesh entities.

These concepts are implemented by the classes MeshEntity, Vertex, Edge, Face, Facet, Cell.

## 3.2 Mesh iterators

Algorithms operating on a mesh can often be expressed in terms of *iterators*. The mesh library provides the general iterator MeshEntityIterator for iteration over mesh entities, as well as the specialized mesh iterators VertexIterator, EdgeIterator, FaceIterator, FaceIterator and Cell-Iterator.

The following code illustrates how to iterate over all incident (connected) vertices of all vertices of all cells of a given mesh:

```
for (CellIterator c(mesh); !c.end(); ++c)
for (VertexIterator v0(*c); !v0.end(); ++v0)
for (VertexIterator v1(*v0); !v1.end(); ++v1)
cout << *v1 << endl;</pre>
```

This may alternatively be implemented using the general iterator MeshEntity-Iterator as follows:

```
unsigned int dim = mesh.topology().dim();
for (MeshEntityIterator c(mesh, dim); !c.end(); ++c)
for (MeshEntityIterator v0(*c, 0); !v0.end(); ++v0)
for (MeshEntityIterator v1(*v0, 0); !v1.end(); ++v1)
cout << *v1 << endl;</pre>
```

# 3.3 Mesh functions

A MeshFunction represents a discrete function that takes a value on each mesh entity of a given topological dimension. A MeshFunction may for example be used to store a global numbering scheme for the entities of a (parallel) mesh, marking sub domains or boolean markers for mesh refinement.

## 3.4 Mesh refinement

A mesh may be refined uniformly as follows:

mesh.refine();

A mesh may also be refined locally by supplying a MeshFunction with boolean markers for the cells that should be refined.

# 3.5 Working with meshes

### 3.5.1 Reading a mesh from file

A mesh may be loaded from a file, either by specifying the file name to the constructor of the class Mesh:

```
Mesh mesh("mesh.xml");
```

or by creating a File object and streaming to a Mesh:

```
File file("mesh.xml");
Mesh mesh;
file >> mesh;
```

A mesh may be stored to file as follows:

File file("mesh.xml"); Mesh mesh; file << mesh;</pre>

The **DOLFIN** mesh XML format has changed in **DOLFIN** version 0.6.3. Meshes in the old XML format may be converted to the new XML format using the script dolfin-convert included in the distribution of **DOLFIN**. For instructions, type dolfin-convert --help.

### 3.5.2 Extracting a boundary mesh

For any given mesh, a mesh of the boundary of the mesh (if any) may be created as follows:

```
BoundaryMesh boundary(mesh);
```

A BoundaryMesh is itself a Mesh of the same geometrical dimension and has the topological dimension of the mesh minus one.

The computation of a boundary mesh may also provide mappings from the vertices of the boundary mesh to the corresponding vertices in the original mesh, and from the cells of the boundary mesh to the corresponding facets of the original mesh:

```
MeshFunction<unsigned int> vertex_map,
MeshFunction<unsigned int> cell_map;
BoundaryMesh boundary(mesh, vertex_map, cell_map);
```

#### 3.5.3 Built-in meshes

**DOLFIN** provides functionality for creating simple meshes, such as the mesh of the unit square and the unit cube. The following code demonstrates how to create a  $16 \times 16$  triangular mesh of the unit square (consisting of  $2 \times 16 \times 16 = 512$  triangles) and a  $16 \times 16 \times 16$  tetrahedral mesh of the unit cube (consisting of  $6 \times 16 \times 16 = 24576$  tetrahedra):

```
UnitInterval mesh1D(16);
UnitSquare mesh2D(16, 16);
UnitCube mesh3D(16, 16, 16);
```

► Developer's note: We could easily add other built-in meshes, like the unit disc, the unit sphere, rectangles, blocks etc. Any contributions are welcome.

### 3.5.4 Creating meshes

Simplicial meshes (meshes consisting of intervals, triangles or tetrahedra) may be constructed explicitly by specifying the cells and vertices of the mesh. A specialized interface for creating simplicial meshes is provided by the class MeshEditor. The following code demonstrates how to create a very simple mesh consisting of two triangles covering the unit square:

```
Mesh mesh;
MeshEditor editor(mesh, CellType::triangle, 2, 2);
```

```
editor.initVertices(4);
editor.initCells(2);
editor.addVertex(0, 0.0, 0.0);
editor.addVertex(1, 1.0, 0.0);
editor.addVertex(2, 1.0, 1.0);
editor.addVertex(3, 0.0, 1.0);
editor.addCell(0, 0, 1, 2);
editor.addCell(1, 0, 2, 3);
editor.close();
```

Note that the **DOLFIN** mesh library is not specialized to simplicial meshes, but supports general collections of mesh entities. However, tools like mesh refinement and mesh editors are currently only available for simplicial meshes.

## **Functions**

► Developer's note: Since this chapter was written, the Function class has seen a number of improvements which are not covered here. Chapter needs to be updated.

The central concept of a function on a domain  $\Omega \subset \mathbb{R}^d$  is modeled by the class Function, which is used in **DOLFIN** to represent coefficients or solutions of partial differential equations.

## 4.1 Basic properties

The following basic properties hold for all Functions:

- A Function can be scalar or vector-valued;
- A Function can be restricted (interpolated) to each local Cell of a Mesh;
- The underlying representation of a Function may vary.

Depending on the actual underlying representation of a Function, it may also be possible to evaluate a Function at any given Point.

#### 4.1.1 Representation

Currently supported representations of Functions include *discrete* Functions, *user-defined* Functions and *constant* Functions. These are discussed in detail below.

#### 4.1.2 Assignment

One Function may be assigned to another Function:

```
Function v;
Function u = v;
```

#### 4.1.3 Components and subfunctions

If a Function is vector-valued, or in general *nested* (mixed), a new Function may be created to represent any given *subsystem* (component) of the original Function, as illustrated by the following example:

```
Function u; // Function with two components
Function u0 = u[0]; // First subsystem (component) of u
Function u1 = u[1]; // First subsystem (component) of u
```

If a Function represents a nested function (one defined in terms of a mixed finite element, see below), then indexing has the effect of picking out subfunctions. With w a Function representing the solution w = (u, p) of a Stokes or Navier-Stokes system (with u the vector-valued velocity and p the scalar pressure), the following example illustrates how to pick subfunctions and components of w:

```
Function w; // Mixed Function (u, p)
u = w[0]; // First subfunction (velocity)
```

p = w[1]; // Second subfunction (pressure) u0 = u[0]; // First component of the velocity u1 = u[1]; // Second component of the velocity u2 = u[2]; // Third component of the velocity

#### 4.1.4 **Output**

A Function can be written to a file in various file formats. To write a Function u to file in VTK format, suitable for viewing in ParaView or MayaVi, create a file with extension .pvd:

File file("solution.pvd");
file << u;</pre>

For further details on available file formats, see Chapter 8.

### 4.2 Discrete functions

A discrete Function is defined in terms of a Vector of degrees of freedom, a Mesh, a local-to-global mapping (DofMap) and a finite element. In particular, a discrete Function is given by a linear combinations of basis functions:

$$v = \sum_{i=1}^{N} v_i \phi_i, \tag{4.1}$$

where  $\{\phi_i\}_{i=1}^N$  is the global basis of the finite element space defined by the Mesh and the finite element, and the nodal values  $\{v_i\}_{i=1}^N$  are given by the values of a Vector.

### 4.3 User-defined functions

In the simplest case, a user-defined Function is just an expression in terms of the coordinates and is typically used for defining source terms and initial conditions. For example, a source term could be given by

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

A user-defined Function may be defined by creating a sub class of Function and overloading the eval() function. The following example illustrates how to create a Function representing the function in (4.2):

```
class Source : public Function
{
  public:
    Source(Mesh& mesh) : Function(mesh) {}
    double eval(const double* x) const
    {
      return x[0]*x[1]*sin(x[2] / DOLFIN_PI);
    }
};
Source f;
```

▶ *Developer's note:* Write about how to define vector-valued functions.

#### 4.3.1 Cell-dependent functions

In some cases, it may be convenient to define a Function in terms of properties of the current Cell. One such example is a Function that at any given point takes the value of the mesh size at that point. The following example illustrates how to create such as Function by overloading the eval() function:

```
class MeshSize : public Function
{
  public:
    MeshSize(Mesh& mesh) : Function(mesh) {}
    double eval(const double* x) const
    {
      return cell().diameter();
    }
};
MeshSize h;
```

Note that the current Cell is only available during assembly and has no meaning otherwise. For example, it is not possible to write the Function h to file.

► Developer's note: Write about predefined special functions like MeshSize and FacetNormal.

### 4.3.2 Simple definition of functions in Python

 $\blacktriangleright$  Developer's note: This is a verbatim copy from the mailing list. It should be edited for the manual.

On Wed, Jun 04, 2008 at 12:44:17PM +0200, Martin Sandve Alnaes wrote: 2008/6/3 Anders Logg <logg@simula.no>: On Tue, Jun 03, 2008 at 11:23:41PM +0200, Martin Sandve Alnaes wrote: >> It's easy with some helper functions I have, I can show you tomorrow. >> It only depends on dolfin::Function (i.e. dolfin.cpp\_Function) and Instant.

```
>
> ok, nice. Maybe we can add the helper functions to assemble.py.
Now you can do things like this:
A = assemble(..., coefficients=[myfunction, 1.23, "sin(x[0])"])
1.23 is wrapped in a cpp_Function (i.e. a constant Function), and
the string is compiled as a C++ dolfin::Function like "v[0] = ...;".
If you want more control over the implementation
(i.e. temporary variables in eval for efficiency, if-checks, etc.)
you can also do this:
code = """
class F: dolfin::Function {
 . . .
};
class G: dolfin::Function {
. . .
};
......
f, g = compile_functions(code, mesh)
Or, if you just want to precompile but don't need anything too fancy:
expressions = ["sin(x[0])",
                         ("a*x[1]", "b*x[0]")]
f, g = compile_functions(expressions, mesh)
assert f.rank() == 0
assert g.rank() == 1
g.a = 1.23
g.b = 3.21
Note that:
- a tuple is interpreted as a vector expression
- a tuple of tuples is interpreted as a matrix expression
- variables like a and b in the strings above are detected
  automatically, but this requires all builtin names to be
  registered in the variable dolfin.compile_functions._builtins,
  which currently contains some common mathematical
```

functions like sqrt, pow, exp, sin, pi etc.

- variables are initialized to 0.0, so use compile\_functions if you need control over variable values.
- assemble also accepts tuples like in compile\_functions
- assemble only calls on instant once independently of the number of string expressions, to reduce compilation time
- Error checks are not extensive!

# **Ordinary differential equations**

► *Developer's note:* This chapter needs to be written. In the meantime, look at the demos in src/demo/ode/ and the base class ODE.

# **Partial differential equations**

► *Developer's note:* This chapter needs to be written. In the meantime, look at the demos in src/demo/pde/.

## Nonlinear solver

**DOLFIN** provides tools for solving nonlinear equations of the form

$$F(u) = 0, \tag{7.1}$$

where  $F : \mathbb{R}^n \to \mathbb{R}^n$ . To use the nonlinear solver, a nonlinear function must be defined. The nonlinear solver is then initialised with this function and a solution computed. The source code for examples of solving nonlinear problems can be found in src/demo/nls.

## 7.1 Nonlinear functions

To solve a nonlinear problem, the user must defined a class which represents the nonlinear function F(u). The class should be derived from the **DOLFIN** class NonlinearFunction. It contains the necessary functions to form the function F(u) and the Jacobian matrix  $J = \partial F/\partial u$ . The precise form of the user defined class will depend on the problem being solved. The structure of a user defined class MyNonlinearFunction is shown below.

```
class MyNonlinearFunction : public NonlinearFunction
{
public:
```

The above class computes the function F(u) and its Jacobian J concurrently. In the future, it will be possible to compute F(u) and J either concurrently or separately.

### 7.2 Newton solver

**DOLFIN** provides tools to solve nonlinear systems using Newton's method and variants of it. The following code solves a nonlinear problem, defined by MyNonlinearFunction using Newton's method.

```
Vector u;
MyNonlinearFunction F;
NewtonSolver newton_solver;
nonlinear_solver.solve(F, x);
```

The maximum number of iterations before the Newton procedure is exited can be set through the **DOLFIN** parameter system, along with the relative and absolute tolerances the residual. This is illustrated below.

```
NewtonSolver nonlinear_solver;
nonlinear_solver.set("Newton maximum iterations", 50);
nonlinear_solver.set("Newton relative tolerance", 1e-10);
nonlinear_solver.set("Newton absolute tolerance", 1e-10);
```

The Newton procedure is considered to have converged when the residual  $r_n$  at iteration n is less than the absolute tolerance or the relative residual  $r_n/r_0$  is less than the relative tolerance. By default, the residual at iteration n is given by

$$r_n = \|F(u_n)\|. (7.2)$$

Computation of the residual in this way can be set by

NewtonSolver newton\_solver; newton\_solver.set("Newton convergence criterion", "residual");

For some problems, it is more appropriate to consider changes in the solution u in testing for convergence. At iteration n, the solution is updated via

$$u_n = u_{n-1} + du_n (7.3)$$

where  $du_n$  is the increment. When using an incremental criterion for convergence, the 'residual' is defined as

$$r_n = \|du_n\|. \tag{7.4}$$

Computation of the incremental residual can be set by

```
NewtonSolver newton_solver;
newton_solver.set("Newton convergence criterion", "incremental");
```

#### 7.2.1 Linear solver

The solution to the nonlinear problems is returned in the vector  $\mathbf{x}$ . By default, the NewtonSolver uses a direct solver to solve systems of linear

equations. It is possible to set the type linear solver to be used when creating a NewtonSolver. For example,

```
NewtonSolver newton_solver(gmres);
```

creates a solver which will use GMRES to solve linear systems. For iterative solvers, the preconditioner can also be selected,

```
NewtonSolver newton_solver(gmres, ilu);
```

The above Newton solver will use GMRES in combination with incomplete LU factorisation.

### 7.2.2 Application of Dirichlet boundary conditions

The application of Dirichlet boundary conditions to finite element problems in the context of a Newton solver requires particular attention. The 'residual' F(u) at nodes where Dirichlet boundary conditions are applied is the equal to difference between the imposed boundary condition value and the current solution u. The function

```
DirichletBC bc;
bc.apply(Matrix& A, Matrix& b, const Matrix& x, const Form& form);
```

applies Dirichlet boundary conditions correctly. For a nonlinear finite element problem, the below code assembles the function F(u) and its Jacobian, and applied Dirichlet boundary conditions in the appropriate manner.

```
class MyNonlinearFunction : public NonlinearFunction
{
public:
```

## 7.3 Incremental Newton solver

Newton solvers are commonly used to solve nonlinear equations in a series of steps. This can be done by building a simple loop around a Newton solver, and is shown in the following code.

```
Function u;
Vector x;
MyNonlinearProblem F(u,x); // Initialise u with the vector x
NewtonSolver nonlinear_solver;
// Solve nonlinear problem in a series of steps
double dt = 1.0; double t = 0.0; double T = 3.0;
while( t < T)
{
t += dt;
nonlinear_solver.solve(F, x);
```

}

Typically, the boundary conditions and/or source terms will be dependent on  ${\tt t}.$ 

## 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;</pre>

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
. m	File::octave	GNU Octave
(.m)	File::matlab	MATLAB

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::octave	out	out	out	out	out
File::matlab	out	out	out	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.

 $\blacktriangleright$  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;</pre>

The same thing can of course be accomplished by

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

on the command-line.

#### 8.2.2 VTK

Data saved in VTK format [9] can be visualized using various packages. The powerful and freely available ParaView [7] is recommended. Alternatively, VTK data can be visualized in MayaVi [3], 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;</pre>
```

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 [4].

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

### 8.2.3 GNU Octave

GNU Octave [5] 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 [6]. (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)

#### 8.2.4 MATLAB

Since MATLAB [2] 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.

### 8.3 Converting between file formats

**DOLFIN** supplies a script for easy conversion between different file formats. The script is named dolfin-convert and can be found in the directory src/utils/convert/ of the **DOLFIN** source tree. The only supported file formats are currently the Medit .mesh format, the Gmsh .msh version 2.0 format and the **DOLFIN** XML (.xml) mesh format.

To convert a mesh in Medit .mesh format generated by TetGen with the -g option, type

# dolfin-convert mesh.mesh mesh.xml

To convert a mesh in Gmsh .msh format type

# dolfin-convert mesh.msh mesh.xml

In generating a Gmsh mesh, make sure to define a physical surface/volume. It is also possible to convert a mesh from the old **DOLFIN** XML (.xml) mesh format to the current one by typing

# dolfin-convert -i xml-old old\_mesh.xml new\_mesh.xml

Example meshes can be found in the directory src/utils/convert/ of the **DOLFIN** source tree.

## 8.4 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.

Also consider contributing to the dolfin-convert script by adding a conversion routine for your favorite format. The script is written in Python and should be easy to extend with new formats.g

## 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 info() available in the dolfin namespace:

```
void info(std::string format, ...);
```

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

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

As an alternative to 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;</pre>
```

Note the use of dolfin::cout and dolfin::endl from the dolfin namespace, corresponding to the standard 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;</pre>

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() displays all matrix entries.

### 9.2 Warnings and errors

Warnings and error messages can be generated using the functions

```
warning(std::string format, ...);
error(std::string format, ...);
```

Once an error is encountered, the program throws an exception.

## 9.3 Debug messages and assertions

The macro dolfin\_debug() works similarly to 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 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:

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():

```
assert(i >= 0);
assert(i < n);
assert(cell.type() == Cell::triangle);
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 begin();
void end();
```

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

```
void begin(std::string format, ...);
void end();
```

These functions enable the **DOLFIN** log system to display messages, warnings and errors hierarchically, by automatically indenting the output produced between calls to begin() and 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;
}</pre>
```

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 )
{
    ...</pre>
```

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":

```
dolfin_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). Messages may also be turned off completely. To specify the destination, set the value of the parameter "output destination":

```
dolfin_set("output destination", "terminal");
dolfin_set("output destination", "silent");
```

One may also set the debug level for the **DOLFIN** log system so that only messages with a debug level higher than or equal to the current debug level are printed:

dolfin\_set("debug level", "1");

## **Parameters**

► Developer's note: Since this chapter was written, the **DOLFIN** parameter system has been completely redesigned and now supports localization of parameters to objects or hierarchies of objects. Chapter needs to be updated.

**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(std::string 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:

```
double 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 small 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++)
{
    ...
}</pre>
```

## **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(std::string key, Parameter value);

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 add() available in the dolfin namespace:

```
void add(std::string key, Parameter value);
```

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

The following examples illustrate the use of add():

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

### **10.4** Saving parameters to file

The following code illustrates how to save the current database of parameters to a file in **DOLFIN** XML format:

```
File file("parameters.xml");
file << ParameterSystem::parameters;</pre>
```

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

The following code illustrates how to load a set of parameters into the current database of parameters from a file in **DOLFIN** XML format:

```
File file("parameters.xml");
file >> ParameterSystem::parameters;
```

The following example illustrates how to specify a list of parameters in the **DOLFIN** XML format

```
<?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

# **PyDOLFIN**

 $\blacktriangleright$  Developer's note: Describe Python interface, especially in areas where it differs from the C++ interface,

## Bibliography

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## **Appendix A**

## **Reference cells**

The definition of reference cells used in **DOLFIN** follows the UFC specification. [14]

The following five reference cells are covered by the UFC specification: the reference *interval*, the reference *triangle*, the reference *quadrilateral*, the reference *tetrahedron* and the reference *hexahedron* (see Table A.1).

The UFC specification assumes that each cell in a finite element mesh is always isomorphic to one of the reference cells.

Reference cell	Dimension	#Vertices	#Facets
The reference interval	1	2	2
The reference triangle	2	3	3
The reference quadrilateral	2	4	4
The reference tetrahedron	3	4	4
The reference hexahedron	3	8	6

Table A.1: Reference cells covered by the UFC specification.

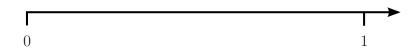


Figure A.1: The reference interval.

Vertex	Coordinate
$v_0$	x = 0
$v_1$	x = 1

Table A.2: Vertex coordinates of the reference interval.

## A.1 The reference interval

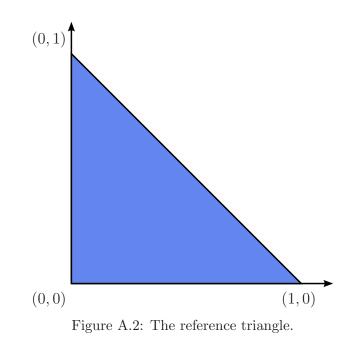
The reference interval is shown in Figure A.1 and is defined by its two vertices with coordinates as specified in Table A.2.

## A.2 The reference triangle

The reference triangle is shown in Figure A.2 and is defined by its three vertices with coordinates as specified in Table A.3.

Vertex	Coordinate
$v_0$	x = (0,0)
$v_1$	x = (1, 0)
$v_2$	x = (0, 1)

Table A.3: Vertex coordinates of the reference triangle.



## A.3 The reference quadrilateral

The reference quadrilateral is shown in Figure A.3 and is defined by its four vertices with coordinates as specified in Table A.4.

Vertex	Coordinate
$v_0$	x = (0, 0)
$v_1$	x = (1, 0)
$v_2$	x = (1, 1)
$v_3$	x = (0, 1)

Table A.4: Vertex coordinates of the reference quadrilateral.

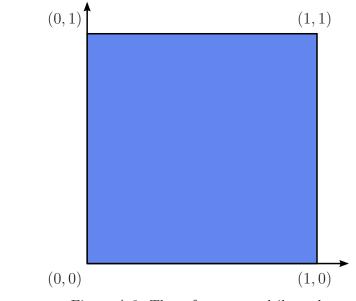


Figure A.3: The reference quadrilateral.

## A.4 The reference tetrahedron

The reference tetrahedron is shown in Figure A.4 and is defined by its four vertices with coordinates as specified in Table A.5.

Vertex	Coordinate
$v_0$	x = (0, 0, 0)
$v_1$	x = (1, 0, 0)
$v_2$	x = (0, 1, 0)
$v_3$	x = (0, 0, 1)

Table A.5: Vertex coordinates of the reference tetrahedron.

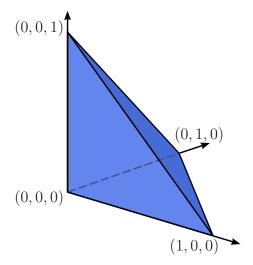


Figure A.4: The reference tetrahedron.

Vertex	Coordinate	Vertex	Coordinate
$v_0$	x = (0, 0, 0)	$v_4$	x = (0, 0, 1)
$v_1$	x = (1, 0, 0)	$v_5$	x = (1, 0, 1)
$v_2$	x = (1, 1, 0)	$v_6$	x = (1, 1, 1)
$v_3$	x = (0, 1, 0)	$v_7$	x = (0, 1, 1)

Table A.6: Vertex coordinates of the reference hexahedron.

## A.5 The reference hexahedron

The reference hexahedron is shown in Figure A.5 and is defined by its eight vertices with coordinates as specified in Table A.6.

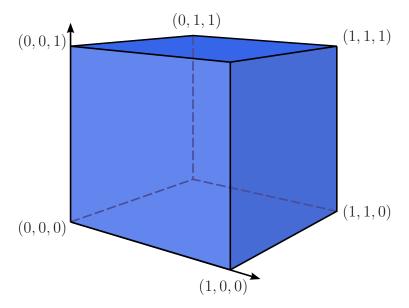


Figure A.5: The reference hexahedron.

## Appendix B

## Numbering of mesh entities

The numbering of mesh entities used in DOLFIN follows the UFC specification [14] for each mesh that has been ordered.<sup>1</sup>

The UFC specification dictates a certain numbering of the vertices, edges etc. of the cells of a finite element mesh. First, an *ad hoc* numbering is picked for the vertices of each cell. Then, the remaining entities are ordered based on a simple rule, as described in detail below.

## **B.1** Basic concepts

The topological entities of a cell (or mesh) are referred to as *mesh entities*. A mesh entity can be identified by a pair (d, i), where d is the topological dimension of the mesh entity and i is a unique index of the mesh entity. Mesh entities are numbered within each topological dimension from 0 to  $n_d - 1$ , where  $n_d$  is the number of mesh entities of topological dimension d.

For convenience, mesh entities of topological dimension 0 are referred to as *vertices*, entities of dimension 1 as *edges*, entities of dimension 2 as *faces*, entities of *codimension* 1 as *facets* and entities of codimension 0 as *cells*.

<sup>&</sup>lt;sup>1</sup>To order a mesh, call the order() function: mesh.order().

Entity	Dimension	Codimension
Vertex	0	_
Edge	1	_
Face	2	_
Facet	_	1
Cell	_	0

Table B.1: Named mesh entities.

These concepts are summarized in Table B.1.

Thus, the vertices of a tetrahedron are identified as  $v_0 = (0,0)$ ,  $v_1 = (0,1)$ and  $v_2 = (0,2)$ , the edges are  $e_0 = (1,0)$ ,  $e_1 = (1,1)$ ,  $e_2 = (1,2)$ ,  $e_3 = (1,3)$ ,  $e_4 = (1,4)$  and  $e_5 = (1,5)$ , the faces (facets) are  $f_0 = (2,0)$ ,  $f_1 = (2,1)$ ,  $f_2 = (2,2)$  and  $f_3 = (2,3)$ , and the cell itself is  $c_0 = (3,0)$ .

### **B.2** Numbering of vertices

For simplicial cells (intervals, triangles and tetrahedra) of a finite element mesh, the vertices are numbered locally based on the corresponding global vertex numbers. In particular, a tuple of increasing local vertex numbers corresponds to a tuple of increasing global vertex numbers. This is illustrated in Figure B.1 for a mesh consisting of two triangles.

For non-simplicial cells (quadrilaterals and hexahedra), the numbering is arbitrary, as long as each cell is isomorphic to the corresponding reference cell by matching each vertex with the corresponding vertex in the reference cell. This is illustrated in Figure B.2 for a mesh consisting of two quadrilaterals.

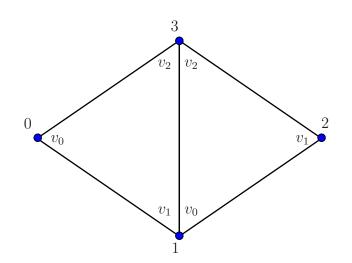


Figure B.1: The vertices of a simplicial mesh are numbered locally based on the corresponding global vertex numbers.

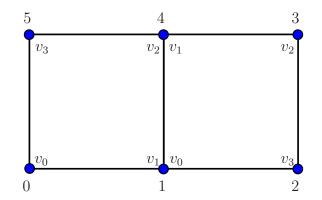


Figure B.2: The local numbering of vertices of a non-simplicial mesh is arbitrary, as long as each cell is isomorphic to the reference cell by matching each vertex to the corresponding vertex of the reference cell.

### **B.3** Numbering of other mesh entities

When the vertices have been numbered, the remaining mesh entities are numbered within each topological dimension based on a *lexicographical ordering* of the corresponding ordered tuples of *non-incident vertices*.

As an illustration, consider the numbering of edges (the mesh entities of topological dimension one) on the reference triangle in Figure B.3. To number the edges of the reference triangle, we identify for each edge the corresponding non-incident vertices. For each edge, there is only one such vertex (the vertex opposite to the edge). We thus identify the three edges in the reference triangle with the tuples  $(v_0)$ ,  $(v_1)$  and  $(v_2)$ . The first of these is edge  $e_0$  between vertices  $v_1$  and  $v_2$  opposite to vertex  $v_0$ , the second is edge  $e_1$  between vertices  $v_0$  and  $v_2$  opposite to vertex  $v_1$ , and the third is edge  $e_2$  between vertices  $v_0$  and  $v_1$  opposite to vertex  $v_2$ .

Similarly, we identify the six edges of the reference tetrahedron with the corresponding non-incident tuples  $(v_0, v_1)$ ,  $(v_0, v_2)$ ,  $(v_0, v_3)$ ,  $(v_1, v_2)$ ,  $(v_1, v_3)$  and  $(v_2, v_3)$ . The first of these is edge  $e_0$  between vertices  $v_2$  and  $v_3$  opposite to vertices  $v_0$  and  $v_1$  as shown in Figure B.4.

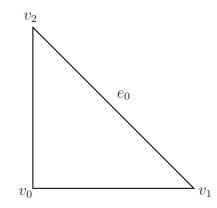


Figure B.3: Mesh entities are ordered based on a lexicographical ordering of the corresponding ordered tuples of non-incident vertices. The first edge  $e_0$  is non-incident to vertex  $v_0$ .

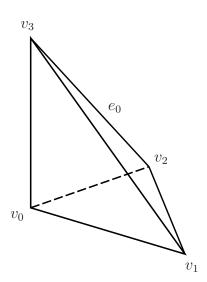


Figure B.4: Mesh entities are ordered based on a lexicographical ordering of the corresponding ordered tuples of non-incident vertices. The first edge  $e_0$  is non-incident to vertices  $v_0$  and  $v_1$ .

#### B.3.1 Relative ordering

The relative ordering of mesh entities with respect to other incident mesh entities follows by sorting the entities by their (global) indices. Thus, the pair of vertices incident to the first edge  $e_0$  of a triangular cell is  $(v_1, v_2)$ , not  $(v_2, v_1)$ . Similarly, the first face  $f_0$  of a tetrahedral cell is incident to vertices  $(v_1, v_2, v_3)$ .

For simplicial cells, the relative ordering in combination with the convention of numbering the vertices locally based on global vertex indices means that two incident cells will always agree on the orientation of incident subsimplices. Thus, two incident triangles will agree on the orientation of the common edge and two incident tetrahedra will agree on the orientation of the common edge(s) and the orientation of the common face (if any). This is illustrated in Figure B.5 for two incident triangles sharing a common edge.

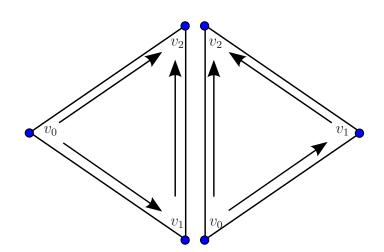


Figure B.5: Two incident triangles will always agree on the orientation of the common edge.

### **B.3.2** Limitations

The UFC specification is only concerned with the ordering of mesh entities with respect to entities of larger topological dimension. In other words, the UFC specification is only concerned with the ordering of incidence relations of the class d - d' where d > d'. For example, the UFC specification is not concerned with the ordering of incidence relations of the class 0 - 1, that is, the ordering of edges incident to vertices.

## **B.4** Numbering schemes for reference cells

The numbering scheme is demonstrated below for cells isomorphic to each of the five reference cells.

#### **B.4.1** Numbering of mesh entities on intervals

Entity	Incident vertices	Non-incident vertices
$v_0 = (0, 0)$	$(v_0)$	$(v_1)$
$v_1 = (0, 1)$	$(v_1)$	$(v_0)$
$c_0 = (1, 0)$	$(v_0, v_1)$	Ø

### B.4.2 Numbering of mesh entities on triangular cells

Entity	Incident vertices	Non-incident vertices
$v_0 = (0, 0)$	$(v_0)$	$(v_1, v_2)$
$v_1 = (0, 1)$	$(v_1)$	$(v_0, v_2)$
$v_2 = (0, 2)$	$(v_2)$	$(v_0, v_1)$
$e_0 = (1, 0)$	$(v_1, v_2)$	$(v_0)$
$e_1 = (1, 1)$	$(v_0, v_2)$	$(v_1)$
$e_2 = (1, 2)$	$(v_0, v_1)$	$(v_2)$
$c_0 = (2,0)$	$(v_0, v_1, v_2)$	Ø

Entity	Incident vertices	Non-incident vertices
$v_0 = (0, 0)$	$(v_0)$	$(v_1, v_2, v_3)$
$v_1 = (0, 1)$	$(v_1)$	$(v_0, v_2, v_3)$
$v_2 = (0, 2)$	$(v_2)$	$(v_0, v_1, v_3)$
$v_3 = (0,3)$	$(v_3)$	$(v_0, v_1, v_2)$
$e_0 = (1, 0)$	$(v_2, v_3)$	$(v_0, v_1)$
$e_1 = (1, 1)$	$(v_1, v_2)$	$(v_0, v_3)$
$e_2 = (1, 2)$	$(v_0, v_3)$	$(v_1, v_2)$
$e_3 = (1,3)$	$(v_0, v_1)$	$(v_2, v_3)$
$c_0 = (2,0)$	$(v_0, v_1, v_2, v_3)$	Ø

### B.4.3 Numbering of mesh entities on quadrilateral cells

### B.4.4 Numbering of mesh entities on tetrahedral cells

Entity	Incident vertices	Non-incident vertices
$v_0 = (0, 0)$	$(v_0)$	$(v_1, v_2, v_3)$
$v_1 = (0, 1)$	$(v_1)$	$(v_0, v_2, v_3)$
$v_2 = (0, 2)$	$(v_2)$	$(v_0, v_1, v_3)$
$v_3 = (0,3)$	$(v_3)$	$(v_0, v_1, v_2)$
$e_0 = (1, 0)$	$(v_2, v_3)$	$(v_0, v_1)$
$e_1 = (1, 1)$	$(v_1, v_3)$	$(v_0, v_2)$
$e_2 = (1, 2)$	$(v_1, v_2)$	$(v_0, v_3)$
$e_3 = (1,3)$	$(v_0, v_3)$	$(v_1, v_2)$
$e_4 = (1, 4)$	$(v_0, v_2)$	$(v_1, v_3)$
$e_5 = (1,5)$	$(v_0, v_1)$	$(v_2, v_3)$
$f_0 = (2, 0)$	$(v_1, v_2, v_3)$	$(v_0)$
$f_1 = (2, 1)$	$(v_0, v_2, v_3)$	$(v_1)$
$f_2 = (2, 2)$	$(v_0, v_1, v_3)$	$(v_2)$
$f_3 = (2,3)$	$(v_0, v_1, v_2)$	$(v_3)$
$c_0 = (3,0)$	$(v_0, v_1, v_2, v_3)$	Ø

Entity	Incident vertices	Non-incident vertices
$v_0 = (0, 0)$	$(v_0)$	$(v_1, v_2, v_3, v_4, v_5, v_6, v_7)$
$v_1 = (0, 1)$	$(v_1)$	$(v_0, v_2, v_3, v_4, v_5, v_6, v_7)$
$v_2 = (0, 2)$	$(v_2)$	$(v_0, v_1, v_3, v_4, v_5, v_6, v_7)$
$v_3 = (0,3)$	$(v_3)$	$(v_0, v_1, v_2, v_4, v_5, v_6, v_7)$
$v_4 = (0, 4)$	$(v_4)$	$(v_0, v_1, v_2, v_3, v_5, v_6, v_7)$
$v_5 = (0, 5)$	$(v_5)$	$(v_0, v_1, v_2, v_3, v_4, v_6, v_7)$
$v_6 = (0, 6)$	$(v_6)$	$(v_0, v_1, v_2, v_3, v_4, v_5, v_7)$
$v_7 = (0,7)$	$(v_7)$	$(v_0, v_1, v_2, v_3, v_4, v_5, v_6)$
$e_0 = (1, 0)$	$(v_6, v_7)$	$(v_0, v_1, v_2, v_3, v_4, v_5)$
$e_1 = (1, 1)$	$(v_5, v_6)$	$(v_0, v_1, v_2, v_3, v_4, v_7)$
$e_2 = (1, 2)$	$(v_4, v_7)$	$(v_0, v_1, v_2, v_3, v_5, v_6)$
$e_3 = (1,3)$	$(v_4, v_5)$	$(v_0, v_1, v_2, v_3, v_6, v_7)$
$e_4 = (1, 4)$	$(v_3, v_7)$	$(v_0, v_1, v_2, v_4, v_5, v_6)$
$e_5 = (1, 5)$	$(v_2, v_6)$	$(v_0, v_1, v_3, v_4, v_5, v_7)$
$e_6 = (1, 6)$	$(v_2, v_3)$	$(v_0, v_1, v_4, v_5, v_6, v_7)$
$e_7 = (1,7)$	$(v_1, v_5)$	$(v_0, v_2, v_3, v_4, v_6, v_7)$
$e_8 = (1, 8)$	$(v_1, v_2)$	$(v_0, v_3, v_4, v_5, v_6, v_7)$
$e_9 = (1, 9)$	$(v_0, v_4)$	$(v_1, v_2, v_3, v_5, v_6, v_7)$
$e_{10} = (1, 10)$	$(v_0, v_3)$	$(v_1, v_2, v_4, v_5, v_6, v_7)$
$e_{11} = (1, 11)$	$(v_0, v_1)$	$(v_2, v_3, v_4, v_5, v_6, v_7)$
$f_0 = (2, 0)$	$(v_4, v_5, v_6, v_7)$	$(v_0, v_1, v_2, v_3)$
$f_1 = (2, 1)$	$(v_2, v_3, v_6, v_7)$	$(v_0, v_1, v_4, v_5)$
$f_2 = (2, 2)$	$(v_1, v_2, v_5, v_6)$	$(v_0, v_3, v_4, v_7)$
$f_3 = (2,3)$	$(v_0, v_3, v_4, v_7)$	$(v_1, v_2, v_5, v_6)$
$f_4 = (2, 4)$	$(v_0, v_1, v_4, v_5)$	$(v_2, v_3, v_6, v_7)$
$f_5 = (2, 5)$	$(v_0, v_1, v_2, v_3)$	$(v_4, v_5, v_6, v_7)$
$c_0 = (3, 0)$	$(v_0, v_1, v_2, v_3, v_4, v_5, v_6, v_7)$	Ø

## B.4.5 Numbering of mesh entities on hexahedral cells

## Appendix C

## Design

This chapter discusses details of the design of **DOLFIN** and is intended mainly for developers of **DOLFIN**.

## C.1 Linear algebra

The linear algebra library provides a uniform interface to uBLAS and PETSc linear algebra through a set of wrappers for basic data structures (matrices and vectors) and solvers, such as Krylov subspace solvers with preconditioners.

For both sets of wrappers, a common interface is defined by the classes GenericMatrix and GenericVector. **DOLFIN** provides a number of algorithms, most notably the assembly algorithms, that work only through the common interface, which means that these algorithms work for any given representation that implements the interface specified by GenericMatrix or GenericVector. A class diagram for the **DOLFIN** linear algebra implementation is given in Figure C.1.

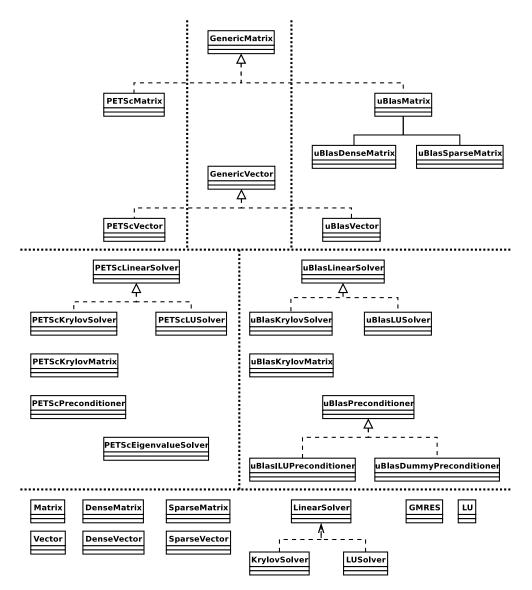


Figure C.1: Class diagram of the linear algebra classes in **DOLFIN**.

## Appendix D

## 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 an effort is underway to provide precompiled Debian packages of **DOLFIN** and other **FENICS** components.

## D.1 Installing from source

#### D.1.1 Dependencies and requirements

**DOLFIN** depends on a number of libraries that need to be installed on your system. These libraries include Boost, Libxml2 and optionally PETSc and

UMFPACK. If you wish to use the Python interface **PyDOLFIN**, the libraries SWIG and NumPy are required. In addition to these libraries, you need to install **FIAT** and **FFC** if you want to define your own variational forms.

#### **Installing Boost**

Boost is a collection of C++ source libraries. Boost can be obtained from

http://www.boost.org/

Packages are available for most Linux distributions. For Ubuntu/Debian users, the package to install is boost-dev.

#### 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 Ubuntu/Debian users, the package to install is libxml2-dev.

#### Installing NumPy

NumPy is required for generating the Python interface **PyDOLFIN**. It can be obtained from

```
http://numpy.scipy.org/
```

Packages are available for most Linux distributions. For Ubuntu/Debian users, the packages python-numpy python-numpy-ext should be installed.

#### Installing SWIG

SWIG is also required for generating the Python interface  $\mathsf{PyDOLFIN}.$  It can be obtained from

http://www.swig.org/

Packages are available for most Linux distributions. For Ubuntu/Debian users, the package swig should be installed.

#### Installing UMFPACK

UMFAPCK is part of the SuiteSparse collection and is a library for the direct solution of linear systems. It is highly recommended if PESTSc is not installed. If PETSc is not installed, UMFPACK is the default direct linear solver. The SuiteSparse collection can be downloaded from

http://www.cise.ufl.edu/research/sparse/SuiteSparse/

UMFPACK is available as a package for many Linux distributions. For Ubuntu/Debian users, the packages libumfpack4 and libumfpack4-dev should be installed. For other distributions, the package may be called libufsparse.

#### Installing PETSc

Optionally, **DOLFIN** may be compiled with support for PETSc. To compile **DOLFIN** with PETSc, add the flag --enable-petsc during the initial configuration of **DOLFIN**.

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 2.3.1, 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), and --download-umfpack=yes to configure.py if you want to install UMFPACK which provided as fast direct linear solver. Both packages are highly recommended.

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 NumPy [11] (Debian package <code>python-numpy</code>) and LinearAlgebra (Debian package <code>python-numpy-ext</code>). Refer to the **FFC** manual for further details.

### D.1.2 Downloading the source code

The latest release of  $\mathsf{DOLFIN}$  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-x.y.z.tar.gz, and unpack using the command

# tar zxfv dolfin-x.y.z.tar.gz

This creates a directory dolfin-x.y.z containing the **DOLFIN** source code.

If you want the very latest version of **DOLFIN**, it can be accessed directly from the development repository through hg (Mercurial):

# hg clone http://www.fenics.org/hg/dolfin

This version may contain features not yet present in the latest release, but may also be less stable and even not work at all.

### D.1.3 Compiling the source code

**DOLFIN** is built using the standard GNU Autotools (Automake, Autoconf) and libtool, 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
# 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 --enable-petsc to compile **DOLFIN** with support for PETSc.
- Use the option --disable-pydolfin to compile without support for PyDOLFIN.
- 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/.

### D.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

### D.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.

### D.2 Debian package

In preparation.

### D.3 Installing from source under Windows

**DOLFIN** can be used under Windows using Cygwin, which provides a Linuxlike environment. The installation process is the same as under GNU/Linux. 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 NumPy is not available as a Cygwin package and must be installed manually. To compile **DOLFIN**, the Cygwin package libxml2-devel must be installed. For **PyDOLFIN** the package swig must be installed. NumPy is not available as a package for Cygwin, therefore it must be installed manually if you wish to use **PyDOLFIN**. The compilation procedure is then the same as under GNU/Linux. If MPI has not been installed:

# ./configure --disable-mpi
# make

followed by an optional

# make install

will compile **DOLFIN** on your system.

## Appendix E

## **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. Patches can be created with Mercurial or diff.

## E.1 Creating bundles/patches

#### E.1.1 Creating a Mercurial (hg) bundle

Creating bundles is the preferred way of submitting patches. It has several advantages over plain diffs. If you are a frequent contributor, consider publishing your source tree so that the **FFC** maintainers (and other users) may pull your changes directly from your tree.

A bundle contains your contribution to **DOLFIN** in the form of a binary patch file generated by Mercurial [10], the revision control system used by **DOLFIN**. Follow the procedure described below to create your bundle.

1. Clone the **DOLFIN** repository:

```
# hg clone http://www.fenics.org/hg/dolfin
```

2. If your contribution consists of new files, add them to the correct location in the **DOLFIN** directory tree. Enter the **DOLFIN** directory and add these files to the local repository by typing:

# hg add <files>

where **<files>** is the list of new files. You do not have to take any action for previously existing files which have been modified. Do not add temporary or binary files.

3. Enter the **DOLFIN** directory and commit your contribution:

# hg commit -m "<description>"

where **<description>** is a short description of what your patch accomplishes.

4. Create the bundle:

```
# hg bundle dolfin-<identifier>-<date>.hg
http://www.fenics.org/hg/dolfin
```

written as one line, where <identifier> is a keyword that can be used to identify the bundle 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.

The bundle now exists as dolfin-<identifier>-<date>.hg.

When you add your contribution at point 2, make sure that only the files that you want to share are present by typing:

# hg status

This will produce a list of files. Those marked with a question mark are not tracked by Mercurial. You can track them by using the add command as shown above. Once you have added these files, their status changes form ? to A.

#### E.1.2 Creating a standard (diff) patch file

The tool used to create a patch is called diff and the tool used to apply the patch is called patch.

Here's an example of how it works. Start from the latest release of **DOLFIN**, which we here assume is release x.y.z. You then have a directory structure under dolfin-x.y.z 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-x.y.z dolfin-x.y.z-mod
```

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

# tar zxfv dolfin-x.y.z.tar.gz

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

```
# ls
dolfin-x.y.z
dolfin-x.y.z-mod
```

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

```
# diff -u --new-file --recursive dolfin-x.y.z
dolfin-x.y.z-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-x.y.z to easily create your modified version. If the patch is large, compressing it with for example gzip is advisable:

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

## E.2 Sending bundles/patches

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

#### dolfin-dev@fenics.org

Include a short description of what your patch/bundle accomplishes. Small patches/bundles 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/bundles if possible.

## E.3 Applying changes

#### **E.3.1** Applying a Mercurial bundle

You have received a patch in the form of a Mercurial bundle. The following procedure shows how to apply the patch to your version of **DOLFIN**.

1. Before applying the patch, you can check its content by entering the **DOLFIN** directory and typing:

```
# hg incoming -p
bundle://<path>/dolfin-<identifier>-<date>.hg
```

written as one line, where <path> is the path to the bundle. <path> can be omitted if the bundle is in the **DOLFIN** directory. The option -p can be omitted if you are only interested in a short summary of the changesets found in the bundle.

2. To apply the patch to your version of **DOLFIN** type:

# hg unbundle <path>/dolfin-<identifier>-<date>.hg

followed by:

# hg update

#### E.3.2 Applying a standard patch file

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

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

```
# tar zxfv dolfin-x.y.z.tar.gz
```

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

```
# ls
dolfin-x.y.z
dolfin-<identifier>-<date>.patch
```

Unpack the patch file using gunzip if necessary.

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

# cd dolfin-x.y.z

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-runwhich can be used to test the patch without actually applying it.

5. The modified version now exists as dolfin-x.y.z.

#### E.4 License agreement

By contributing a patch to **DOLFIN**, you agree to license your contributed code under the GNU Lesser General Public License (a condition also built into the LGPL 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 LGPL Version 2.1.
//
// 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 F

# Contributors

► Developer's note: List all contributors here.

# Appendix G

# **Coding style**

To streamline the **DOLFIN** source code and ease the job for maintainers that need to read and edit large amounts of code, developers should try to follow the below coding style when submitting patches to **DOLFIN**.

The guideline below is for C++ but may in some cases be extrapolated to Python.

## G.1 Naming conventions

#### G.1.1 Class names

Use camel caps for class names:

```
class FooBar
{
    ...
};
```

#### G.1.2 Function names

Use lower-case for function names and underscore to separate words:

void foo(); void bar(); void foo\_bar(...);

Functions returning a value should be given the name of that value, for example:

```
class Array:
{
  public:
    /// Return size of array (number of entries)
    uint size() const;
};
```

In the above example, the function should be named **size** rather than **get\_size**. On the other hand, a function not returning a value but rather taking a variable (by reference) and assigning a value to it, should use the **get\_foo** naming scheme, for example:

```
class Parameters:
{
  public:
    /// Retrieve all parameter keys
    void get_parameter_keys(std::vector<std::string>& parameter_keys) const;
};
```

#### G.1.3 Variable names

Use lower-case for variable names and underscore to separate words:

Foo foo; Bar bar; FooBar foo\_bar;

#### G.1.4 Enum variables and constants

Enum variables should be lower-case with underscore to separate words:

enum Type {foo, bar, foo\_bar};

We try to avoid using **#define** to define constants, but when necessary constants should be capitalized:

#define FOO 3.14159265358979

#### G.1.5 File names

Use camel caps for file names if they contain the declaration/definition of a class. Header files should have the suffix .h and implementation files should have the suffix .cpp:

FooBar.h FooBar.cpp

Use lower-case for file names that contain utilities/functions (not classes).

## G.2 Miscellaneous

#### G.2.1 Comments

Comment your code, and do it often. Capitalize the first letter and don't use punctuation (unless the comment runs over several sentences). Here's a good example from TopologyComputation.cpp:

```
// Check if connectivity has already been computed
if (connectivity.size() > 0)
return;
// Invalidate ordering
mesh._ordered = false;
// Compute entities if they don't exist
if (topology.size(d0) == 0)
computeEntities(mesh, d0);
if (topology.size(d1) == 0)
computeEntities(mesh, d1);
// Check if connectivity still needs to be computed
if (connectivity.size() > 0)
return;
...
```

#### G.2.2 Integers and reals

Use dolfin::uint instead of int (unless you really want to use negative integers which is rare) and dolfin::real instead of double:

uint i = 0; double x = 0.0;

These are typedefs for the standard C++ types unsigned int and double (defined in dolfin/common/types.h).

#### G.2.3 Placement of brackets

Curly brackets following a control statement should appear in the next line and not be indented:

for (uint i = 0; i < 10; i++)
{
 ...
}</pre>

#### G.2.4 Indentation

Indentation should be two spaces and it should be spaces, not tab(s).

#### G.2.5 Header file layout

Header files should follow the below template:

```
// Copyright (C) 2008 Foo Bar.
// Licensed under the GNU LGPL Version 2.1.
//
// Modified by Bar Foo, 2008.
//
// First added: 2008-01-01
// Last changed: 2008-02-01
```

```
#ifndef __FO0_H
#define __FO0_H
namespace dolfin
{
    class Bar; // Forward declarations here
    /// Documentation of class
    class Foo
    {
        public:
        ...
        private:
        ...
    };
}
#endif
```

#### G.2.6 Implementation file layout

Implementation files should follow the below template:

```
// Copyright (C) 2008 Foo Bar.
// Licensed under the GNU LGPL Version 2.1.
//
// Modified by Bar Foo, 2008.
```

```
11
// First added: 2008-01-01
// Last changed: 2008-02-01
#include <dolfin/Foo.h>
using namespace dolfin;
//-----
Foo::Foo() : // variable initialization here
{
 . . .
}
//-----
Foo::~Foo()
{
 // Do nothing
}
      _____
//-----
```

The horizontal lines above should be exactly 79 characters wide but have been shortened here to fit the page.

## G.2.7 Including header files

Don't use **#include** <dolfin.h> or **#include** <dolfin/dolfin\_foo.h> inside the DOLFIN kernel. Only include the portions of DOLFIN you are actually using.

## G.2.8 Forward declarations

Actually, try to include as little as possible and use forward declarations whenever possible (in header files). Put the **#include** in the implementation file.

#### G.2.9 Explicit constructors

Make all constructors (except copy constructors) explicit if there is no particular reason not to do so:

```
class Foo
{
    explicit Foo(uint i);
};
```

### G.2.10 Virtual functions

Always declare inherited virtual functions as virtual in the subclasses. This makes it easier to spot which functions are virtual.

```
class Foo
{
   virtual void foo();
   virtual void bar() = 0;
};
class Bar
{
   virtual void foo();
   virtual void bar();
};
```

## G.3 Use of libraries

## G.3.1 Prefer C++ strings and streams to old C-style char\*

Use std::string instead of const char\* and use std::istream and std::ostream instead of FILE. Avoid printf, sprintf and the like.

There are exceptions to this rule where we need to use old C-style function calls. One such exception is handling of command-line arguments (char\* argv[]).

## **Appendix H**

## License

**DOLFIN** is licensed under the GNU Lesser General Public License (LGPL) version 2.1, included verbatim below.

GNU LESSER GENERAL PUBLIC LICENSE Version 2.1, February 1999

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[This is the first released version of the Lesser GPL. It also counts as the successor of the GNU Library Public License, version 2, hence the version number 2.1.]

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We call this license the "Lesser" General Public License because it does Less to protect the user's freedom than the ordinary General Public License. It also provides other free software developers Less of an advantage over competing non-free programs. These disadvantages are the reason we use the ordinary General Public License for many libraries. However, the Lesser license provides advantages in certain special circumstances.

For example, on rare occasions, there may be a special need to encourage the widest possible use of a certain library, so that it becomes a de-facto standard. To achieve this, non-free programs must be allowed to use the library. A more frequent case is that a free library does the same job as widely used non-free libraries. In this case, there is little to gain by limiting the free library to free software only, so we use the Lesser General Public License.

In other cases, permission to use a particular library in non-free programs enables a greater number of people to use a large body of free software. For example, permission to use the GNU C Library in non-free programs enables many more people to use the whole GNU operating system, as well as its variant, the GNU/Linux operating system.

Although the Lesser General Public License is Less protective of the users' freedom, it does ensure that the user of a program that is linked with the Library has the freedom and the wherewithal to run that program using a modified version of the Library.

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"Source code" for a work means the preferred form of the work for making modifications to it. For a library, complete source code means all the source code for all modules it contains, plus any associated interface definition files, plus the scripts used to control compilation and installation of the library.

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a) The modified work must itself be a software library.

b) You must cause the files modified to carry prominent notices stating that you changed the files and the date of any change.

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