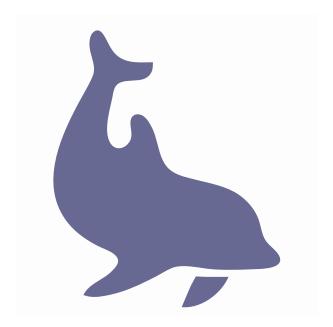
November 15, 2006



Visit http://www.fenics.org/ for the latest version of this manual. Send comments and suggestions to dolfin-dev@fenics.org.

Contents

\mathbf{A}	bout	this m	nanual	8
1	Qui	ckstart	t	11
	1.1	Downl	loading and installing DOLFIN	11
	1.2	Solvin	g Poisson's equation with DOLFIN	12
		1.2.1	Setting up the variational formulation	13
		1.2.2	Writing the solver	14
		1.2.3	Compiling the program	19
		1.2.4	Running the program	20
		1.2.5	Visualizing the solution	20
2	Line	ear alg	ebra	23
	2.1	Matrio	ces and vectors	23
		2.1.1	Sparse matrices	25
		2.1.2	Dense matrices	25

D	OLFII	V User	Manual	Н	off	m	ar	١,	Ja	ıns	SSO	on	,	Lo	gg	٣,	W	ells
		2.1.3	The common interface															26
	2.2	Solvin	g linear systems															26
		2.2.1	Iterative methods															26
		2.2.2	Direct methods															28
	2.3	Solvin	g eigenvalue problems															29
	2.4	Linear	algebra backends															30
		2.4.1	uBlas															30
		2.4.2	PETSc															30
9	ml	ala																ก1
3	1 ne	mesh																31
	3.1	Basic	concepts															32
		3.1.1	Mesh															32
		3.1.2	Mesh entities															32
	3.2	Mesh	iterators															33
	3.3	Mesh	functions															33
	3.4	Mesh	refinement															34
	3.5	Worki	ng with meshes															34
		3.5.1	Reading a mesh from file															34
		3.5.2	Extracting a boundary mesh															35
		3.5.3	Built-in meshes															35

DOI		11	N / I
1)()1	FII/I	User	Manual

Fun	ctions		37
4.1	Basic	properties	37
	4.1.1	Representation	38
	4.1.2	Evaluation	38
	4.1.3	Assignment	39
	4.1.4	Components and sub functions	39
	4.1.5	Output	40
4.2	Discre	ete functions	40
	4.2.1	Creating a discrete function	41
	4.2.2	Accessing discrete function data	42
	4.2.3	Attaching discrete function data	42
4.3	User-c	defined functions	43
	4.3.1	Creating a sub class	43
	4.3.2	Specifying a function-pointer	45
	4.3.3	Cell-dependent functions	45
4.4	Time-	dependent functions	46
Ord	linary	differential equations	47
Par	tial di	fferential equations	49
Nor	nlinear	solver	51
	4.1 4.2 4.3 Par	4.1.1 4.1.2 4.1.3 4.1.4 4.1.5 4.2 Discrete 4.2.1 4.2.2 4.2.3 4.3 4.3 User-o 4.3.1 4.3.2 4.3.3 4.4 Time- Ordinary Partial discrete 4.1.1 4.1.2 4.2.2 4.2.3 4.3.1	4.1 Basic properties 4.1.1 Representation 4.1.2 Evaluation 4.1.3 Assignment 4.1.4 Components and sub functions 4.1.5 Output 4.1 Discrete functions 4.2.1 Creating a discrete function 4.2.2 Accessing discrete function data 4.2.3 Attaching discrete function data 4.3 User-defined functions 4.3.1 Creating a sub class 4.3.2 Specifying a function-pointer 4.3.3 Cell-dependent functions

וחח	Haar	Manual
	11861	iviaiiiiai

	7.1	Nonlinear functions	51
	7.2	Newton solver	52
		7.2.1 Linear solver	53
		7.2.2 Application of Dirichlet boundary conditions	54
	7.3	Incremental Newton solver	55
8	Inp	ut/output	57
	8.1	Files and objects	57
	8.2	File formats	59
		8.2.1 DOLFIN XML	59
		8.2.2 VTK	60
		8.2.3 OpenDX	61
		8.2.4 GNU Octave	61
		8.2.5 MATLAB	62
		8.2.6 GiD	62
	8.3	Converting between file formats	63
	8.4	A note on new file formats	63
9	The	log system	65
	9.1	Generating log messages	65
	9.2	Warnings and errors	66
	9.3	Debug messages and assertions	67

D O I			
DOL	.HIN	User	Manual

	9.4	Task notification	68
	9.5	Progress bars	69
	9.6	Controlling the destination of output	70
10	Para	ameters	73
	10.1	Retrieving the value of a parameter	73
	10.2	Modifying the value of a parameter	74
	10.3	Adding a new parameter	75
	10.4	Saving parameters to file	76
	10.5	Loading parameters from file	76
11	Solv	rers	77
		erence elements	77 81
	Refe		81
	Refe	erence elements	81 81
	Refe	erence elements The reference triangle	81 81 83
	Refe	The reference tetrahedron	81818384
	Refe	The reference triangle	81 81 83 84 84
	Refe	The reference triangle	81 83 84 84 87
	Refe	The reference triangle	81 83 84 84 87

_	\sim	 			
ı	m	NI	User	NASE	บบาไ
ப	VIL	 14	USEL	iviai	шаі

		A.3.6	Alignment of faces	88
В	Des	ign		91
	B.1	Linear	algebra	91
\mathbf{C}	Inst	allatio	n	93
	C.1	Installi	ing from source	93
		C.1.1	Dependencies and requirements	93
		C.1.2	Downloading the source code	96
		C.1.3	Compiling the source code	96
		C.1.4	Compiling the demo programs	98
		C.1.5	Compiling a program against DOLFIN	98
	C.2	Debiar	ı package	99
	C.3	Install	ing from source under Windows	99
D	Con	.tributi	ing code	101
	D.1	Creati	ng a patch	101
	D.2	Sendin	g patches	103
	D.3	Applyi	ing a patch (maintainers)	103
	D.4	License	e agreement	104
${f E}$	Lice	ense		105

About this manual

This manual is currently being written. As a consequence, some sections may be incomplete or inaccurate.

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 C 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 0.1.0 of **DOLFIN**:

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

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

Note that you may need to be root on your system to perform the last step. Since **DOLFIN** depends on a number of other packages, you may also need to download and install these packages before you can compile **DOLFIN**. (See Appendix C 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 $\Gamma_0 = \{(x,y) \in \partial\Omega : x=0\}$, the Neumann boundary condition $\partial_n u = 1$ on the boundary $\Gamma_1 = \{(x,y) \in \partial\Omega : x=1\}$, homogeneous Neumann boundary conditions on the remaining part of the boundary and right-hand side given by $f(x,y) = 500 \exp(-((x-0.5)^2 + (y-0.5)^2)/0.02)$, corresponding to a source localized at x=y=0.5:

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

$$u(x,y) = 0, (x,y) \in \Gamma_0 = \{(x,y) \in \partial\Omega : x = 0\},$$
 (1.2)

$$\partial_n u(x,y) = 1, \quad (x,y) \in \Gamma_1 = \{(x,y) \in \partial\Omega : x = 1\},$$
 (1.3)

$$\partial_n u(x,y) = 0, \quad (x,y) \in \partial\Omega \setminus (\Gamma_0 \cup \Gamma_1).$$
 (1.4)

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

$$a(v, U) = L(v) \quad \forall v \in \hat{V}_h,$$
 (1.5)

¹To install **DOLFIN** locally on a normal user account, configure **DOLFIN** to use another installation directory, for example ./configure --prefix=~/local. Alternatively, you may use the command ./configure.local to install **DOLFIN** locally in a subdirectory of the source tree.

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

$$a(v, U) = \int_{\Omega} \nabla v \cdot \nabla U \, dx \tag{1.6}$$

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

$$L(v) = \int_{\Omega} v f \, dx + \int_{\partial \Omega} v g \, ds, \qquad (1.7)$$

where $g = \partial_n u$ is the Neumann boundary condition.

1.2.1 Setting up the variational formulation

The variational formulation (1.5) must be given to **DOLFIN** as a pair of bilinear and linear forms (a, L) using the form compiler **FFC**. This is done by entering the definition of the forms in a text file with extension .form, e.g. Poisson.form, as follows:

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

v = TestFunction(element)
U = TrialFunction(element)
f = Function(element)
g = Function(element)

a = dot(grad(v), grad(U))*dx
L = v*f*dx + v*g*ds
```

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 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 (1.5) 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 <code>src/demo/pde/poisson/</code> of the **DOLFIN** source tree.

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

```
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 and 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
{
   real eval(const Point& p, unsigned int i)
   {
     real dx = p.x - 0.5;
     real dy = p.y - 0.5;
     return 500.0*exp(-(dx*dx + dy*dy)/0.02);
   }
};
```

The Dirichlet boundary condition is specified similarly, by overloading the eval() function for a subclass of BoundaryCondition:

```
class DirichletBC : public BoundaryCondition
{
  void eval(BoundaryValue& value, const Point& p, unsigned int i)
  {
    if ( std::abs(p.x - 0.0) < DOLFIN_EPS )
      value = 0.0;
  }
};</pre>
```

The Neumann boundary conditions is specified as a Function that gets integrated over the boundary $\partial\Omega$ of Ω :

```
class NeumannBC : public Function {
```

```
real eval(const Point& p, unsigned int i)
{
   if ( std::abs(p.x - 1.0) < DOLFIN_EPS )
     return 1.0;
   else
     return 0.0;
}
</pre>
```

We may now create the right-hand side, the Dirichlet and the Neumann boundary conditions as follows:

```
Source f;
DirichletBC bc;
NeumannBC g;
```

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

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

Next, we initialize the pair of bilinear and linear forms that we have previously compiled with **FFC**:

```
Poisson::BilinearForm a;
Poisson::LinearForm L(f, g);
```

Note that the right-hand side f and the Neumann boundary condition g need to be given as arguments to the constructor of the linear form, since the linear form depends on these two functions.

We may now define a PDE from the pair of forms, the mesh and the Dirichlet boundary condition:

```
PDE pde(a, L, mesh, bc);
```

To solve the PDE, we now just need to call the solve function as follows:

```
Function U = pde.solve();
```

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;

int main()
{
    // Right-hand side
    class Source : public Function
    {
       real eval(const Point& p, unsigned int i)
       {
            real dx = p.x - 0.5;
            real dy = p.y - 0.5;
            return 500.0*exp(-(dx*dx + dy*dy)/0.02);
       }
```

```
};
// Dirichlet boundary condition
class DirichletBC : public BoundaryCondition
  void eval(BoundaryValue& value, const Point& p, unsigned int i)
    if ( std::abs(p.x - 0.0) < DOLFIN_EPS )
      value = 0.0;
  }
};
// Neumann boundary condition
class NeumannBC : public Function
  real eval(const Point& p, unsigned int i)
    if ( std::abs(p.x - 1.0) < DOLFIN_EPS )
      return 1.0;
    else
      return 0.0;
  }
};
// Set up problem
Source f;
DirichletBC bc;
NeumannBC g;
UnitSquare mesh(16, 16);
Poisson::BilinearForm a;
Poisson::LinearForm L(f, g);
PDE pde(a, L, mesh, bc);
// Compute solution
Function U = pde.solve();
// Save solution to file
File file("poisson.pvd");
file << U;
```

```
return 0;
}
```

1.2.3 Compiling the program

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

With the Makefile in place, we just need to type make to compile the program, generating the executable as the file dolfin-poisson. Note that this requires that the script dolfin-config is in your PATH. During make install of **DOLFIN**, this script will be automatically generated and placed in the subdirectory bin of the installation directory you have chosen for **DOLFIN**, which means you need to make sure this subdirectory is in your PATH.²

²You will be reminded of this during the initial configuration of **DOLFIN**.

1.2.4 Running the program

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

```
# ./dolfin-poisson
Computing mesh connectivity:
Found 289 vertices
Found 512 cells
[...]
Solving linear system of size 289 x 289 (UMFPACK LU solver).
Saved function u (no description) to file poisson.pvd [...]
```

1.2.5 Visualizing the solution

DOLFIN relies on external programs for visualization. In this example, we chose to save the solution in VTK format, which can be imported into for example ParaView or MayaVi. A simple way to visualize the computed solution is to run the Python script plot.py which is present in the directory of the Poisson demo (and most other demos):

```
python plot.py
```

This script calls MayaVi to visualize the solution.

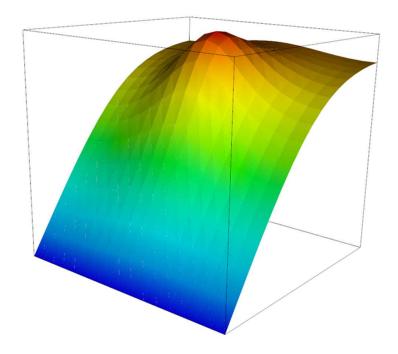


Figure 1.1: The solution of Poisson's equation (1.1) visualized in MayaVi.

Chapter 2

Linear algebra

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 a wrappers that provide a common interface to the functionality of the linear algebra libraries uBlas [13] and PETSc [10].

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;

real a = A(4, 3);

x(3) = 2.0;

real 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:

```
real 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:

```
real 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 Matrix¹.

If **DOLFIN** has been compiled with support for PETSc, then the sparse matrix is represented as a sparse PETSc matrix². 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.

2.1.2 Dense matrices

DOLFIN provides the class <code>DenseMatrix</code> 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 (and solving linear systems with a direct solver) is more efficient with a dense matrix representation.

¹The class Matrix is a typedef for the class SparseMatrix.

²By default, the sparse matrix is represented as a PETSc MATSEQAIJ matrix, but other PETSc representations are also available.

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.

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 available)	
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 Solving 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 zeroth eigenpair:

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

The real and complex components of the eigenvalue are returned in lr and lc, respectively, and the real 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 second eigenpair:

```
PETScEigenvalueSolver esolver;
esolver.solve(A, B);

real 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.

Chapter 3

The mesh

- ▶ Developer's note: The **DOLFIN** mesh library has recently been reimplemented from scratch and replaces the old mesh library starting at **DOLFIN** version 0.6.3. The new mesh is simpler, faster and more general than the old mesh library, but adaptive mesh refinement is still missing from the old feature set. This will be added in the near future.
- ▶ 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 CellIterator.

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 MeshEntityIterator 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();
```

DOLFIN does currently not support adaptive mesh refinement, but this will be supported in future versions.

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 16×16 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 $6 \times 16 \times 16 \times 16 = 24576$ tetrahedra):

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

▶ Developer's note: We could easily add other built-in meshes, like the unit interval, 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 evaluated at each Vertex of a Mesh;
- A Function can be restricted 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 and *user-defined* Functions. These are discussed in detail below.

4.1.2 Evaluation

All Functions can be evaluated at the Vertices of a Mesh. The following example illustrates how to evaluate a scalar Function at each Vertex of a given Mesh:

If the Function is vector-valued, an additional argument is needed to specify the component. The following example illustrates how to evaluate all components of a vector-valued Function at all each Vertex of a given Mesh:

If allowed by the underlying representation, a Function u may also be evaluated directly at any given Point:

```
Point p(0.5, 0.5, 0.5);
cout << ''Value at p = '' << p << '': '' << u(p) << endl;
```

As in the case of evaluation at a Vertex, the component index may be given as an additional argument for a vector-valued Function.

4.1.3 Assignment

One Function may be assigned to another Function:

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

Assignment creates a new Function sharing the same data. In particular, this means that modifying the data of one of the two Functions will also affect the other Function.

4.1.4 Components and sub functions

If a Function is vector-valued, a new Function may be created to represent any given component of the original Function, as illustrated by the following example:

If a Function represents a mixed function (one defined in terms of a mixed FiniteElement, see below), then indexing has the effect of picking out sub functions. 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 sub functions and components of w:

```
Function w; // mixed Function (u, p)
u = w[0]; // first sub function (velocity)
p = w[1]; // second sub function (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
```

Note that picking a component or sub function creates a new Function that shares data with the original Function.

4.1.5 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 nodal values (degrees of freedom), a Mesh and a FiniteElement specifying the distribution of the

nodal values on the Mesh. 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 FiniteElement, and the nodal values $\{v_i\}_{i=1}^N$ are given by the values of a Vector.

Note that a *discrete* Function may not be evaluated at arbitrary points (only at each Vertex of a Mesh).

4.2.1 Creating a discrete function

A discrete Function can be initialized in several ways. In the simplest case, only a Vector x of nodal values needs to be specified:

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

If possible, **DOLFIN** will then automatically try to determine the Mesh and the FiniteElement.

In some cases, it is necessary to also supply a Mesh when initializing a discrete Function:

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

If possible, **DOLFIN** will then automatically try to determine the FiniteElement.

In general however, a discrete Function must be initialized from a given Vector, a Mesh and a FiniteElement:

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

4.2.2 Accessing discrete function data

It is possible to access the data of a discrete Function, including the associated Vector, Mesh and FiniteElement:

```
Vector& x = u.vector();
Mesh& mesh = u.mesh();
FiniteElement& element = u.element();
```

4.2.3 Attaching discrete function data

After a discrete Function has been initialized, it is possible to associate or reassociate data with the Function:

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

Function u(x);
u.attach(mesh);
u.attach(element);
```

Usually, the FiniteElement is given by the BilinearForm defining the problem. Considering the Poisson example in Chapter 1, a Function u representing the solution can be initialized as follows:

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

Poisson::BilinearForm a;

FiniteElement& element = a.trial();
u.attach(element);
```

In this example, the Function u represents a function in the trial space for the BilinearForm a.

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

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

There are two ways to create a user-defined Function; either by creating a sub class of Function or by creating a Function from a given function pointer.

4.3.1 Creating a sub class

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
{
   real eval(const Point& p, unsigned int i)
   {
     return x*y*sin(z / DOLFIN_PI);
   }
};
Source f;
```

To create a vector-valued Function, the vector dimension must be supplied to the constructor of Function:

```
class Source : public Function
{
  public:

    Source() : Function(3) {}

    real eval(const Point& p, unsigned int i)
    {
        if ( i == 0 )
            return 0.0;
        else if ( i == 1 )
            return x*y*sin(z / DOLFIN_PI);
        else
            return x + y;
        }
    };
Source f;
```

4.3.2 Specifying a function-pointer

A user-defined Function may alternatively be defined by specifying a function pointer. The following example illustrates an alternative way of creating a Function representing the function in (4.2):

```
real source(const Point& p, unsigned int i)
{
  return x*y*sin(z / DOLFIN_PI);
}
Function f(source);
```

As before, for vector-valued Functions, the vector dimension must be supplied to the constructor of Function:

```
real source(const Point& p, unsigned int i)
{
  if ( i == 0 )
    return 0.0;
  else if ( i == 1 )
    return x*y*sin(z / DOLFIN_PI);
  else
    return x + y;
}
Function f(source, 3);
```

4.3.3 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
{
   real eval(const Point& p, unsigned int i)
   {
     return cell().diameter();
   }
}
MeshSize h;
```

Note that the current Cell is only available during assembly and has no meaning otherwise. It is thus not possible to write the Function h to file, since the current Cell is not available when evaluating a Function at any given Vertex. Furthermore, note that the current Cell is not available when creating a Function from a function pointer.

4.4 Time-dependent functions

▶ Developer's note: Write about time-dependent and pseudo time-dependent functions.

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

$$F(u) = 0, (7.1)$$

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.

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

$$r_n = ||du_n||. (7.4)$$

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 used 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

```
void FEM::applyResidualBC(GenericVector& b,
const GenericVector& x, Mesh& mesh,
FiniteElement& element, BoundaryCondition& bc)
```

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
{
```

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.

```
MyNonlinearProblem F(U);
NewtonSolver nonlinear_solver;

Vector& x = U.vector();

// Solve nonlinear problem in a series of steps real dt = 1.0; real t = 0.0; real T = 3.0; while( t < T) {
    t += dt;</pre>
```

```
nonlinear_solver.solve(F, x);
}
```

Typically, the boundary conditions and/or source terms will be dependent on 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
.dx	File::opendx	OpenDX
.m	File::octave	GNU Octave
(.m)	File::matlab	MATLAB
.msh/.res	File::gid	GiD

Table 8.1: File formats and corresponding file name suffixes.

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

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

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

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

8.2 File formats

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

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

8.2.1 DOLFIN XML

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

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

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

```
in >> mesh;
File out(''mesh.xml'');
out << mesh;</pre>
```

The same thing can of course be accomplished by

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

on the command-line.

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

8.2.2 VTK

Data saved in VTK format [11] can be visualized using various packages. The powerful and freely available ParaView [9] is recommended. Alternatively, VTK data can be visualized in MayaVi [4], 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 [5].

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

8.2.3 OpenDX

OpenDX [8] is a powerful free visualization tool based on IBM's *Visualization Data Explorer*. To visualize data with OpenDX, a user needs to build a *visual program* that instructs OpenDX how to extract and visualize relevant parts of your data. **DOLFIN** provides a ready-made visual program suitable for visualization of **DOLFIN** data in OpenDX. The visual program can be found in the subdirectory src/utils/opendx/ of the **DOLFIN** source tree (file dolfin.net and accompanying configuration dolfin.cfg).

8.2.4 GNU Octave

GNU Octave [6] 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 [7]. (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 <code>poisson.m</code>, then just type

```
octave:1> poisson
```

The solution can now be visualized using the command

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

or to visualize just the mesh, type

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

8.2.5 **MATLAB**

Since MATLAB [3] is not free, users are encouraged to use GNU Octave whenever possible. That said, data is visualized in much the same way in MATLAB as in GNU Octave, using the MATLAB commands pdemesh, pdesurf and pdeplot.

8.2.6 GiD

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

8.3 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 (which can be generated by TetGen) and the **DOLFIN** XML mesh format:

dolfin-convert mesh.mesh mesh.xml

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 <code>src/kernel/io/</code> of the **DOLFIN** source tree to get a feeling for how to design the file format, or ask at <code>dolfin-dev@fenics.org</code> 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.

The log system

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

9.1 Generating log messages

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

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

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

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

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

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

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

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

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

9.2 Warnings and errors

Warnings and error messages can be generated using the macros

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

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

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

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

9.3 Debug messages and assertions

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

```
dolfin_debug(message);
```

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

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

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

```
dolfin_assert(check);
```

This macro accepts a boolean expression and if the expression evaluates to false, an error message is displayed, including the file, function name and line number of the assertion, and a segmentation fault is raised (to enable easy attachment to a debugger). The following examples illustrate the use of dolfin_assert():

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

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

9.4 Task notification

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

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

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

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

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

9.5 Progress bars

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

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

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

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

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

```
p = i;
}
```

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

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

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). Other options include directing messages to a curses interface or turning of messages completely. To specify the output destination, use the function dolfin_output() available in the dolfin namespace:

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

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

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

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

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

Chapter 10

Parameters

▶ 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 get() available in the dolfin namespace:

```
Parameter 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 get() to a variable, as illustrated by the following examples:

```
real TOL = get(''tolerance'');
int num_samples = get(''number of samples'');
bool solve_dual = get(''solve dual problem'');
std::string filename = 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 = 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 **set()** available in the **dolfin** namespace:

```
void 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 set():

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

Note that changing the values of parameters using 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

Chapter 11

Solvers

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

Bibliography

```
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```

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Appendix A

Reference elements

A.1 The reference triangle

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

$$v^{0} = (0,0),$$

 $v^{1} = (1,0),$
 $v^{2} = (0,1).$ (A.1)

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

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

$$e^{0}:(v^{1},v^{2}),$$

 $e^{1}:(v^{2},v^{0}),$
 $e^{2}:(v^{0},v^{1}).$ (A.2)

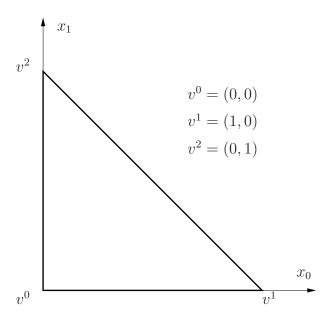


Figure A.1: Physical coordinates of the reference triangle.

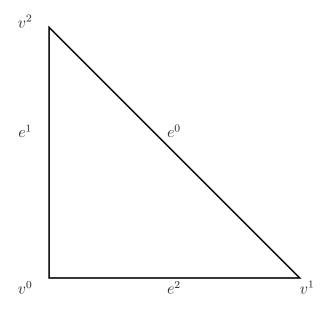


Figure A.2: Ordering of mesh entities (vertices and edges) for the reference triangle.

A.2 The reference tetrahedron

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

$$v^{0} = (0, 0, 0),$$

$$v^{1} = (1, 0, 0),$$

$$v^{2} = (0, 1, 0),$$

$$v^{4} = (0, 0, 1).$$
(A.3)

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

$$f^{0}:(v^{1}, v^{3}, v^{2}),$$

$$f^{1}:(v^{2}, v^{3}, v^{0}),$$

$$f^{2}:(v^{3}, v^{1}, v^{0}),$$

$$f^{3}:(v^{0}, v^{1}, v^{2}).$$
(A.4)

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

$$e^{0}: (v^{1}, v^{2}),$$

$$e^{1}: (v^{2}, v^{0}),$$

$$e^{2}: (v^{0}, v^{1}),$$

$$e^{3}: (v^{0}, v^{3}),$$

$$e^{4}: (v^{1}, v^{3}),$$

$$e^{5}: (v^{2}, v^{3}).$$
(A.5)

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

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

$$f^{0}: (e^{5}, e^{0}, e^{4}),$$

$$f^{1}: (e^{3}, e^{1}, e^{5}),$$

$$f^{2}: (e^{2}, e^{3}, e^{4}),$$

$$f^{3}: (e^{0}, e^{1}, e^{2}).$$
(A.6)

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

A.3 Ordering of degrees of freedom

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

A.3.1 Mesh entities

We distinguish between mesh entities of different topological dimensions:

vertices	topological dimension 0
edges	topological dimension 1
faces	topological dimension 2
cells	topological dimension 2 or 3

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

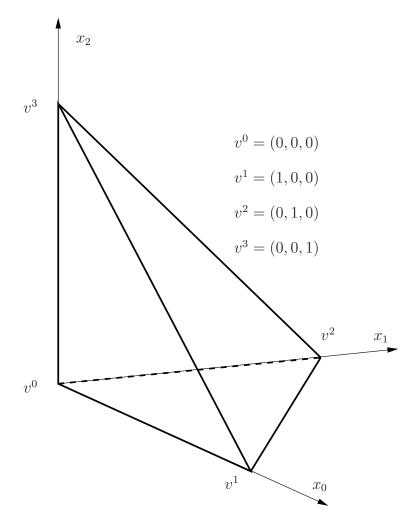


Figure A.3: Physical coordinates of the reference tetrahedron.

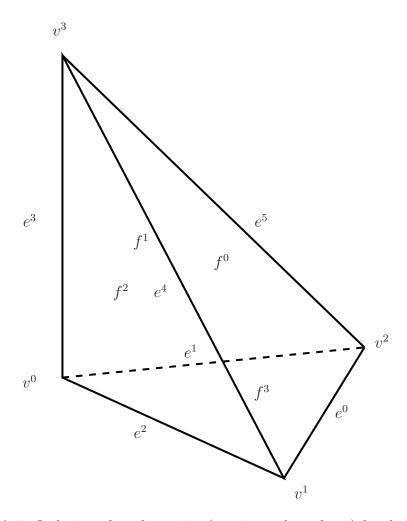


Figure A.4: Ordering of mesh entities (vertices, edges, faces) for the reference tetrahedron.

A.3.2 Ordering among mesh entities

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

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

A.3.3 Internal ordering on edges

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

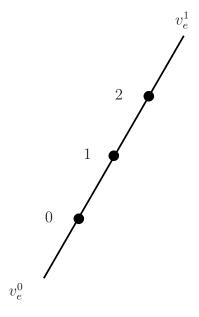


Figure A.5: Internal ordering of nodes on edges.

A.3.4 Alignment of edges

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

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

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

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

A.3.5 Internal ordering on faces

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

A.3.6 Alignment of faces

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

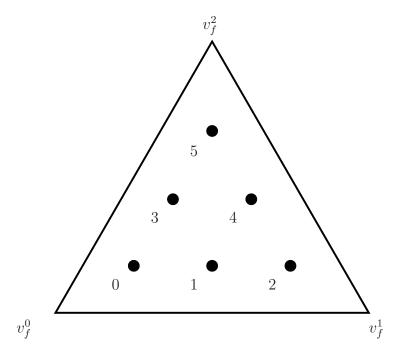


Figure A.6: Internal ordering of nodes on faces.

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

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

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

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

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

Appendix B

Design

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

B.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 B.1.

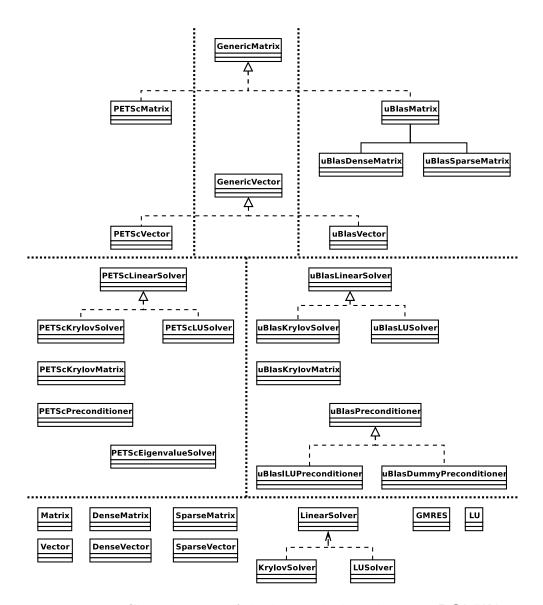


Figure B.1: Class diagram of the linear algebra classes in **DOLFIN**.

Appendix C

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.

C.1 Installing from source

C.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. 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 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 Numeric (Debian package python-numeric) and LinearAlgebra (Debian package python-numeric-ext). Refer to the **FFC** manual for further details.

C.1.2 Downloading the source code

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

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

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

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

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

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

C.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 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/.

C.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 <code>src/demo/</code> of the **DOLFIN** source tree. Just enter the directory containing the demo program you want to compile and type <code>make</code>. You may also compile all demo programs at once using the command

make demo

C.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.

C.2 Debian package

In preparation.

C.3 Installing from source under Windows

DOLFIN can be used under Windows using Cygwin, which provides a Linux-like 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 Numeric is not available as a Cygwin package and must be installed manually. To compile **DOLFIN**, the Cygwin package libxml2-devel must be installed. 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 ${f DOLFIN}$ on your system.

Appendix D

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.

D.1 Creating a patch

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

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

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

```
# make clean
```

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

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

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

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

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

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

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

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

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

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

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

D.2 Sending patches

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

```
dolfin-dev@fenics.org
```

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

D.3 Applying a patch (maintainers)

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

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

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

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

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

Unpack the patch file using gunzip if necessary.

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

```
# cd dolfin-0.1.0
```

4. Apply the patch:

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

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

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

D.4 License agreement

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

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

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

Appendix E

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Index

File, 57 GMRES, 26 GenericMatrix, 26 GenericVector, 26 KrylovSolver, 26 LUSolver, 28 LU, 28	compiling, 96, 98 conjugate gradient method, 27 contact, 10 contributing, 101 curses interface, 70 Cygwin, 99
Matrix, 23	Debian package, 99
Progress, 69	debugging, 67
Vector, 23	demo programs, 98
add(), 75	dense matrix, 25
cout, 65	dependencies, 93
dolfin_assert(), 67	diff, 101
dolfin_begin(), 68	direct methods, 28
dolfin_debug(), 67	downloading, 11, 96
dolfin_end(), 68	
dolfin_error(), 66	eigenvalue problems, 29
$dolfin_info(), 65$	eigenvalue solver, 29
dolfin_log(), 70	enumeration, 10
dolfin_output(), 70	errors, 66
dolfin_warning(), 66	FFC, 95
endl, 65	•
get(), 73	ffc, 13 FIAT, 96
set(), <mark>74</mark>	file formats, 59
1 1 . 1. 1. 1. 1. 1.	Function, 37
algebraic multigrid, 27	functions, 37
AMG, 27	runctions, 37
assertions, 67	GMRES method, 26
BiCGStab, 27	GNU General Public License, 105
Boost, 94	GPL, 105
	- 1 - 0 0

DOLFIN User Manual

reference tetrahedron, 83 reference triangle, 81 SLEPc, 29 SOR, 27 rource code, 96 reparse matrix, 25 ruccessive over-relaxation, 27 asks, 68 rypographic conventions, 9 aBlas, 30 aser-defined functions, 43 rirtual matrix, 28 rvarnings, 66 KML, 59, 76
SLEPc, 29 SOR, 27 SOR, 27 SOURCE code, 96 Sparse matrix, 25 Successive over-relaxation, 27 sasks, 68 suppographic conventions, 9 suBlas, 30 ser-defined functions, 43 virtual matrix, 28 varnings, 66
SLEPc, 29 SOR, 27 cource code, 96 cparse matrix, 25 cuccessive over-relaxation, 27 asks, 68 ypographic conventions, 9 aBlas, 30 aser-defined functions, 43 virtual matrix, 28 varnings, 66
SOR, 27 source code, 96 sparse matrix, 25 successive over-relaxation, 27 asks, 68 ypographic conventions, 9 aBlas, 30 aser-defined functions, 43 virtual matrix, 28 warnings, 66
SOR, 27 source code, 96 sparse matrix, 25 successive over-relaxation, 27 asks, 68 ypographic conventions, 9 aBlas, 30 aser-defined functions, 43 virtual matrix, 28 warnings, 66
ource code, 96 parse matrix, 25 puccessive over-relaxation, 27 asks, 68 ypographic conventions, 9 aBlas, 30 aser-defined functions, 43 virtual matrix, 28 varnings, 66
parse matrix, 25 puccessive over-relaxation, 27 asks, 68 pypographic conventions, 9 aBlas, 30 puser-defined functions, 43 prirtual matrix, 28 pyronings, 66
ypographic conventions, 9 Blas, 30 user-defined functions, 43 virtual matrix, 28 varnings, 66
nBlas, 30 nser-defined functions, 43 virtual matrix, 28 varnings, 66
virtual matrix, 28 varnings, 66
virtual matrix, 28 varnings, 66
virtual matrix, 28 varnings, 66
varnings, 66
varnings, 66
ζ ML, 59, 76
XML, 59, 76