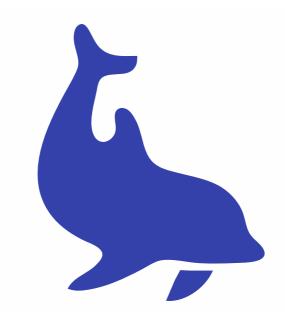
September 23, 2005



Hoffman, Jansson, Logg

www.fenics.org

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### **About this manual**

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

#### Intended audience

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

### **Typographic conventions**

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

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

### **Enumeration and list indices**

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

### **Contact**

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

dolfin-dev@fenics.org

## Introduction

**FIXME:** Automation of CMM, FEniCS, purpose of DOLFIN: PSE for differential equations, C++ interface of FEniCS, etc

### 1.1 The FEniCS project

FIXME: Automation of CMM, other components of FENICS

#### 1.2 The finite element method

**FIXME:** Automation of discretization

### 1.3 Overview

FIXME: Component diagram, user, module, kernel

FIXME: Write about real, uint, namespace dolfin

# Quickstart

- 2.1 Downloading DOLFIN
- 2.2 Installing DOLFIN
- 2.3 Solving Poisson's equation with DOLFIN

# Linear algebra

**DOLFIN** uses PETSc for the linear algebra. For convenience **DOLFIN** provide wrappers for some of the most common linear algebra functionality.

#### 3.1 The Matrix class

The matrix class represents a matrix of dimension m x n. It is a simple wrapper for a PETSc matrix Mat. The interface is intentionally simple. For advanced usage, access the PETSc Mat pointer using the function mat() and use the standard PETSc interface.

#### 3.2 The VirtualMatrix class

This class represents a matrix-free matrix of dimension m x m. It is a simple wrapper for a PETSc shell matrix. The interface is intentionally simple. For advanced usage, access the PETSc Mat pointer using the function mat() and use the standard PETSc interface.

The class VirtualMatrix enables the use of Krylov subspace methods for lin-

ear systems Ax = b, without having to explicitly store the matrix A. All that is needed is that the user-defined VirtualMatrix implements multiplication with vectors. Note that the multiplication operator needs to be defined in terms of PETSc data structures (Vec), since it will be called from PETSc.

#### 3.3 The Vector class

The vector class represents a vector of dimension n. It is a simple wrapper for a PETSc vector Vec. The interface is intentionally simple. For advanced usage, access the PETSc Vec pointer using the function vec() and use the standard PETSc interface.

#### 3.4 The LinearSolver class

This class defines the interface of all linear solvers for systems of the form Ax = b.

#### 3.5 The GMRES class

This class implements the GMRES method for linear systems of the form Ax = b. It is a wrapper for the GMRES solver of PETSc.

#### 3.6 The LU class

This class implements the direct solution (LU factorization) for linear systems of the form Ax = b. It is a wrapper for the LU solver of PETSc.

### 3.7 The EigenvalueSolver class

This class computes eigenvalues of a matrix. It is a wrapper for the eigenvalue solver of PETSc.

#### 3.8 The Preconditioner class

This class specifies the interface for user-defined Krylov method preconditioners. A user wishing to implement her own preconditioner needs only supply a function that approximately solves the linear system given a right-hand side.

### 3.9 The PETScManager class

This class is responsible for initializing and (automatically) finalizing PETSc. To initialize PETSc, call PETScManager::init() once (additional calls will be ignored). Finalization will be handled automatically.

### 3.10 The PETSc system

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.

### 3.11 The Hypre system

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

To use a preconditioner from Hypre with your PETSc solver in **DOLFIN**, write

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

In particular, the above preconditioner boomeramg is an algebraic multigrid preconditioner, which may be very useful for some problems.

**FIXME:** Write about the wrappers, PETSc, using mat() and vec() to do more advanced operations with PETSc etc.

# **Functions**

**FIXME:** Discuss the Function class and the different representations.

# The mesh

**FIXME:** Triangular, tetrahedral, include some images, mesh refinement, connectivity, iterators, file formats, local ordering

# **Ordinary differential equations**

**FIXME:** Mono-adaptive, multi-adaptive, ODE base class, simple example, error control, adaptivity, complex ODE, implicit, homotopies

# Partial differential equations

### 7.1 Boundary value problems

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

$$-\Delta u(x) = f(x) \quad x \in \Omega \subset \mathbb{R}^d$$

$$u(x) = 0 \quad x \in \partial\Omega.$$
(7.1)

### 7.2 Variational formulation

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

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

where  $a(\cdot, \cdot): V \times V \to \mathbb{R}$  is a bilinear form on V defined by

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

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

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

 $V = H_0^1(\Omega)$  is the standard Sobolev space of square integrable functions with also their first derivatives square integrable (in the Lebesgue sense), with the functions being zero on the boundary (in the sense of traces).

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

$$a(U, v) = L(v) \quad \forall v \in V_h,$$
 (7.5)

where  $V_h \subset V$  is a finite dimensional subspace of dimension N. The finite element space  $V_h$  is characterized by the set of basis functions  $\{\varphi_i\}_{i=1}^N$ , and thus the FEM method (7.5) is specified by the variational form and the basis functions of  $V_h$ .

### 7.3 Compiling the variational form with FFC

In **DOLFIN** a PDE is defined in variational form using tensor notation in a .form file, which is compiled using FFC.

At /dolfin/src/demo/solvers/poisson/dolfin/ the following poisson.form file for (7.5) can be found

```
# Copyright (C) 2005 Johan Hoffman and Anders Logg.
# Licensed under the GNU GPL Version 2.
#
# First added: 2005-04-04
# Last changed: 2005
#
# The bilinear form a(u,v) and linear form L(v) for # Poisson's equation.
#
# Compile this form with FFC: ffc poisson.form.
```

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

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

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

Compiling the file with

# ffc Poisson.form
```

generate a file Poisson.h containing the classes BilinearForm and LinearForm, and classes for the finite element used in the forms.

#### 7.4 The FEM class

The FEM class automates the assembly algorithm, constructing a linear system of equations from a given partial differential equation, specified as a variational problem (7.2), by a bilinear form  $a(\cdot,\cdot)$  and a linear form  $L(\cdot)$ , according to

The assemble function is called in the following way

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

where A and b is a matrix and vector respectively.

#### 7.5 The BilinearForm class

BilinearForm represents a bilinear form a(u, v) with arguments v and u basis functions of the finite element space defined by a pair of finite elements (test and trial).

This class is automatically generated by FFC when compiling the variational form.

The function used in the assembly algorithm is an eval function

```
/// Compute element matrix (interior contribution)
virtual void eval(real block[], const AffineMap& map) const;
```

where the element matrix is returned in block[], and map is describes the affine map used for mapping the reference element to the actual element.

### 7.6 The LinearForm class

LinearForm represents a linear form L(v) with argument v (the test function) a basis function of the finite element space defined by a finite element.

This class is automatically generated by FFC when compiling the variational form.

The function used in the assembly algorithm is an eval function

```
/// Compute element vector (interior contribution)
virtual void eval(real block[], const AffineMap& map) const;
```

where the element vector is returned in block[], and map is describes the affine map used for mapping the reference element to the actual element.

### 7.7 The AffineMap class

This class represents the affine map from the reference element to the current element.

The 2D reference element is given by (0,0)-(1,0)-(0,1). The 3D reference element is given by (0,0,0)-(1,0,0)-(0,1,0)-(0,0,1).

The dimension d of the map is automatically determined from the arguments used when calling the map.

The map is initialized by the function

```
/// Update map for current element
void update(const Cell& cell);
```

When update is called the following local variables in the class are computed for the current cell

```
// Determinant of Jacobian of map
real det;

// Jacobian of map
real f00, f01, f02, f10, f11, f12, f20, f21, f22;

// Inverse of Jacobian of map
real g00, g01, g02, g10, g11, g12, g20, g21, g22;
```

#### 7.8 The FiniteElement class

This is the base class for finite elements automatically generated by FFC.

```
/// Return dimension of the finite element space
virtual unsigned int spacedim() const = 0;
```

#### 7.9 The PDE class

A PDE represents a (linearized) partial differential equation, given by a bilinear form a and a linear form L.

```
/// Constructor
PDE(BilinearForm& a, LinearForm& L);
```

# 7.10 Computation of Element matrices and vectors

divide element matrix into geometry tensor and integration over reference element FErari

precomputation of integrals, quadrature, tensor representation factored out,  $\ensuremath{\mathrm{FFC}}$ 

### 7.11 Boundary conditions

### 7.12 Finite elements

Finite Element by Ciarlet, FIAT

### 7.13 Initial value problems

semidiscretization, space-time FEM,

# Input/output

### 8.1 Pre- and post-processing

FIXME: DOLFIN relies on external programs for pre- and post-processing

### 8.2 Files and objects

**FIXME:** Discuss operators >> and <<

### 8.3 File formats

**FIXME:** Insert table here of filename suffixes and corresponding formats.

#### 8.3.1 DOLFIN XML

**FIXME:** The native format

- 8.3.2 Another format
- 8.3.3 Another format
- 8.3.4 Another format
- 8.4 Adding a new file format

FIXME: Discuss classes File, GenericFile etc

# 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;</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() 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++)
{
    ...
    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 )
{
    ...
    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**

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

## 10.1 Retrieving the value of a parameter

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

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

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

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

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

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

```
int num_samples = dolfin_get(''number of samples'');
for (int i = 0; i < num_samples; i++)
{
    ...
}</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(const char* key, ...);
```

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

The following examples illustrate the use of dolfin\_set():

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

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

## 10.3 Adding a new parameter

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

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

Possible values for type are

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

The following examples illustrate the use of dolfin\_parameter():

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

## 10.4 Saving parameters to file

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

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

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

## 10.5 Loading parameters from file

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

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

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

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

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

# Chapter 11

# **Solvers**

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

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

A solver for a PDE should provide the following interface:

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

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

## 11.1 Poisson's equation

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

$$-\Delta u = f \text{ in } \Omega,$$

$$u = g_D \text{ on } \Gamma_1,$$

$$-\partial_n u = 0 \text{ on } \Gamma_2$$
(11.1)

The variational formulation is given by

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

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

## 11.1.1 Usage

The API for the Poisson solver:

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

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

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

A simple example of using the solver:

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

   PoissonSolver::solve(mesh, f, bc);
   return 0;
}
```

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

### 11.1.2 Performance

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

#### 11.1.3 Limitations

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

### 11.2 Convection-diffusion

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

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

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

The variational formulation is:

#### FIXME: Stabilized convection-diffusion

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

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

### 11.2.1 Usage

The API for the convection-diffusion solver:

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

// Solve convection-diffusion
void solve();

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

A simple example of using the solver:

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

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

   ConvectionDiffusionSolver::solve(mesh, w, f, bc);
   return 0;
}
```

#### 11.2.2 Performance

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

#### 11.2.3 Limitations

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

## 11.3 Incompressible Navier-Stokes

Write introduction here, equations etc.

### 11.3.1 Usage

Present API of solver and give an example.

#### 11.3.2 Performance

Write something about the performance of the solver.

### 11.3.3 Limitations

Write something about the limitations of the solver.

## 11.4 Elasticity

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

$$u = x - X,$$

$$\dot{u} - v = 0 \quad \text{in } \Omega^{0},$$

$$\dot{v} - \nabla \cdot \sigma = f \quad \text{in } \Omega^{0},$$

$$\sigma = E\epsilon(u) = E(\nabla u^{\top} + \nabla u)$$

$$E\epsilon = \lambda tr(\epsilon)I + 2\mu\epsilon,$$

$$v(0, \cdot) = v^{0}, \quad u(0, \cdot) = u^{0} \quad \text{in } \Omega^{0},$$

$$u = g_{D} \quad \text{on } \Gamma_{1} \times (0, T],$$

$$-\partial_{n}u = 0 \quad \text{on } \Gamma_{2} \times (0, T]$$

The variational form:

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

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

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

## 11.4.1 Usage

Present API of solver and give an example.

### 11.4.2 Performance

Write something about the performance of the solver.

### 11.4.3 Limitations

Write something about the limitations of the solver.

# 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)

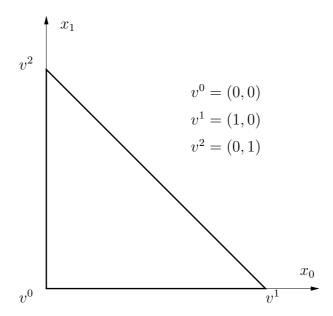


Figure A.1: Physical coordinates of the reference triangle.

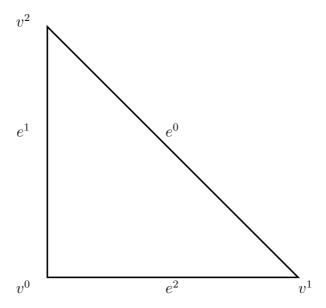


Figure A.2: Ordering of mesh entities (vertices and edges) for the reference triangle.

### 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.

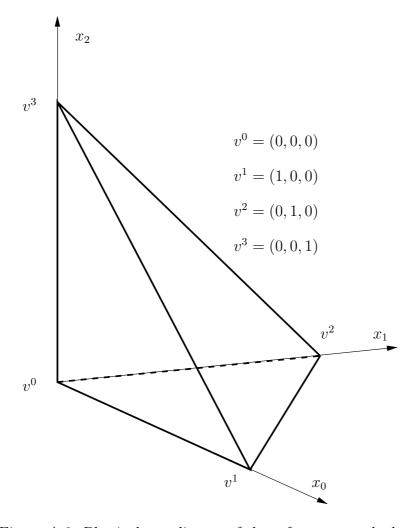


Figure A.3: Physical coordinates of the reference tetrahedron.

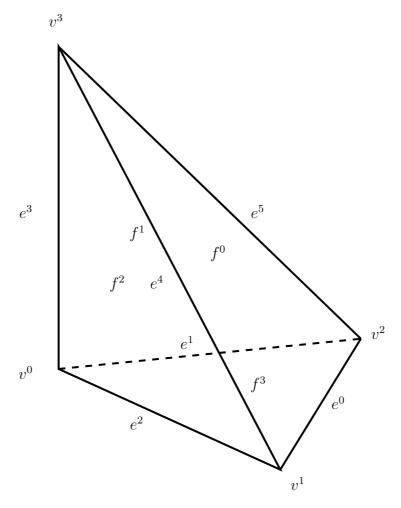


Figure A.4: Ordering of mesh entities (vertices, edges, faces) for the reference tetrahedron.

### 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 lign up.

### A.3.3 Internal ordering on edges

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

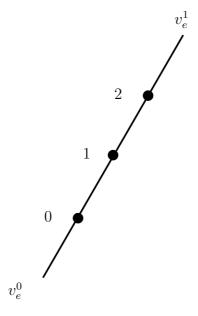


Figure A.5: Internal ordering of nodes on edges.

### A.3.4 Alignment of edges

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

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

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

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

### A.3.5 Internal ordering on faces

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

## A.3.6 Alignment of faces

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

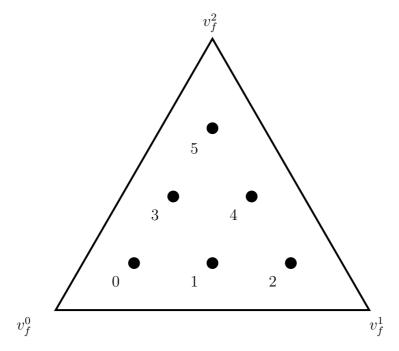


Figure A.6: Internal ordering of nodes on faces.

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

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

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

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

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

# Appendix B

# Installation

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

dolfin-dev@fenics.org

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

## **B.1** Installing from source

## **B.1.1** Dependencies and requirements

**DOLFIN** depends on a number of libraries that need to be installed on your system. These libraries include Libxml2 and PETSc. In addition to these libraries, you need to install **FIAT** and **FFC** if you want to define your own variational forms.

#### **Installing Libxml2**

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

```
http://xmlsoft.org/
```

For Debian users, the package to install is libxml2-dev.

#### **Installing PETSc**

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

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

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

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

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

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

#### Installing FFC

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

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

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

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

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

### B.1.2 Downloading the source code

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

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

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

```
# tar 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.

### B.1.3 Compiling the source code

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

```
# ./configure
```

# make

followed by an optional

# make install

to install **DOLFIN** on your system.

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

# ./configure --help

for a complete list of arguments.

• Use the option --prefix=<path> to specify an alternative directory for installation of **DOLFIN**. The default directory is /usr/local/, which means that header files will be installed under /usr/local/inlude/ and libraries will be installed under /usr/local/lib/. This option can be useful if you don't have root access but want to install **DOLFIN** locally on a user account as follows:

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

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

### **B.1.4** Compiling the demo programs

After compiling the **DOLFIN** library according to the instructions above, you may want to try one of the demo programs in the subdirectory <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

## B.1.5 Compiling a program against DOLFIN

Whether you are writing your own Makefiles or using an automated build system such as GNU Autotools or BuildSystem, it is straightforward to compile a program against **DOLFIN**. The necessary include and library paths

can be obtained through the script dolfin-config which is automatically generated during the compilation of **DOLFIN** and installed in the bin subdirectory of the <path> specified with --prefix. Assuming this directory is in your executable path (environment variable PATH), the include path for building **DOLFIN** can be obtained from the command

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

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

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

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

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

## B.2 Debian package

In preparation.

# Appendix C

# **Contributing code**

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

## C.1 Creating a patch

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

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

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

- # make clean
- 2. From the parent directory, rename the **DOLFIN** directory to something else:

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

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

```
# tar 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
```

## C.2 Sending patches

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

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

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

#### C.3 Applying a patch (maintainers)

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

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

```
# tar 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.

#### C.4 License agreement

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

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

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

## Appendix D

### License

**DOLFIN** is licensed under the GNU General Public License (GPL) version 2, included verbatim below.

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