# Draft on Dune-Fem-Functionals

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#### Abstract

This document is a draft about a new concept of DUNE-FEM based on functionals. DUNE-FEM is part of the Distributed and Unified Numerics Environment (DUNE) and is available from http://dune.mathematik.uni-freiburg.de/.

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# 1 Introduction

The overall goal of Dune-Fem and Dune-Fem-Functionals is the efficient numerical solution of PDE's. Assuming standard notation, the following elliptic PDE may serve as a sample problem.

Example 1.1 (Elliptic PDE in one dimension).

Let  $\Omega \subset \mathbb{R}$  be a domain and  $a, f : \Omega \to \mathbb{R}$  and  $g : \partial\Omega \to \mathbb{R}$  be given functions.

Find  $u: \Omega \to \mathbb{R}$ , such that

$$-\nabla \cdot (a\nabla u) = f \qquad in \Omega,$$

$$u = g \qquad on \partial\Omega.$$
(1.1)

## **Definition 1.2.** Weak formulation

Let  $H^1$  and  $H^1_0$  be given as usual and let  $H^1_g$  for  $g \in H^1$  be defined as

$$H_g^1 := \{ v \in H^1 | v = w + g \text{ for } a w \in H_0^1 \}.$$

The weak formulation of problem (1.1) then reads as follows. Find  $u \in H_g^1$ , such that

$$\int_{\Omega} a \nabla u \nabla v \, dx = \int_{\Omega} f v \, dx \qquad \qquad for \ all \ v \in H_0^1. \tag{1.2}$$

The weak formulation (1.2) gives rise to the introduction of functionals and operators. A rigorous mathematical definition of these can be found in the next section. The following is only intended to give the basic idea.

#### **Definition 1.3** (Operators and functionals).

The function f from he original problem 1.1 induces a functional

$$F: H_0^1 \to \mathbb{R}$$
$$v \mapsto F[v] := \int_{\Omega} fv \, dx.$$

Accordingly the function a from the original problem 1.1 induces an operator

$$A: H_g^1 \to H^{-1}$$
$$u \mapsto A(u),$$

where A(u) itself is a functional, defined by

$$A(u): H_0^1 \to \mathbb{R}$$
 
$$v \mapsto A(u)[v] := \int_{\Omega} a \nabla u \nabla v \, dx.$$

With these definitions at hand the weak formulation (1.2) can be rewritten in the following way.

**Remark 1.4** (Variational formulation using functionals and operator). Let A and F be as in definition 1.3. The weak formulation (1.2) can be rewritten as follos. Find  $u \in H_g^1$ , such that

$$A(u)[v] = F[v] \qquad \qquad for \ all \ v \in H_0^1. \tag{1.3}$$

Our postulate is, that a wide range of interesting problems can be written in this form. For detailed examples of linear and nonlinear problems see section?.

# 2 Abstract concept

We start with an overview on the mathematical concept which is carried over to a corresponding programming concept. The following notations and definitions are required for the subsequent sections.

# **Definition 2.1** (Function and Functionspace).

Let  $n, d \in \mathbb{N}^{\geq 1}$  be integers and  $\Omega \subseteq \mathbb{R}^n$  a subset. A mapping  $v : \Omega \to \mathbb{R}^d$  is called a function, the set

$$V := \{v : \Omega \to \mathbb{R}^d\}$$

is called a function space. If V is an  $\mathbb{R}$ -vector space, V is called a linear function space.

#### **Definition 2.2** (Functional).

Let V be a function space. A map

$$F: V \to \mathbb{R},$$

$$v \mapsto F[v] \tag{2.1}$$

is called a Functional. If

$$F[\alpha v_1 + \beta v_2] = \alpha F[v_1] + \beta F[v_2]$$

holds for all  $\alpha, \beta \in \mathbb{R}$  and all  $v_1, v_2 \in V$ , F is called a linear Functional. The vector space

$$V' := \{ F : V \to \mathbb{R} | F \text{ is a linear functional } \}$$
 (2.2)

is called the dual space of V.

# Lemma 2.3 (Localization property of discrete linear functionals).

Let  $V_G$  be a discrete function space ([1, Def. 18]) and  $F \in V_G^*$  a discrete linear functional. Let further be

$$u = \sum_{E \in G} u_E \tag{2.3}$$

the representation for a  $u \in V_G$  in terms of its local functions  $u_E := u_{|E}$  and

$$u_E = \sum_{i \in I_E} u_i^E \varphi_i^E \tag{2.4}$$

the representation of a local function in terms of its local DoFs  $u_i^E$  and the local base functions  $\varphi_i^E$  ([1, Def. 20]). Thus,  $u_E$  can be written as

$$u = \sum_{E \in G} \sum_{i \in I_E} u_{\mu_G(i)}^E \varphi_{\mu_G(i)}^E,$$

where  $\mu_G$  is local-to-global DoF mapping ([1, Def. 18]). Since F if a discrete linear functional, it holds that

$$F[u] = \sum_{E \in G} \sum_{i \in I_E} u_{\mu_G(i)}^E F\left[\varphi_{\mu_G(i)}^E\right], \tag{2.5}$$

which can also be written as

$$F[u] = \sum_{E \in G} u^E \cdot F[B_E]^E, \tag{2.6}$$

where  $u^E := (u^E_{\mu_G(i)})_{i \in I_E}$  is the local DoF vector of  $u_E$  (mapped to global) and  $F[B_E]^E$  is defined as the vector

$$F[B_E]^E := \left( F \left[ \varphi_{\mu_G(i)}^E \right] \right)_{i \in I_E} \tag{2.7}$$

for a local basfunction set  $B_E$ .

#### **Definition 2.4** (Constraint).

Let V be a linear function space,  $M \in \mathbb{N}_{>0}$  and  $\{F_1, ..., F_M\}$  a set of linear functionals on V. We define the corresponding vector of linear functionals C by

$$C: \{1, ..., M\} \times V \to \mathbb{R} \text{ with } (i, v) \mapsto C[i][v] := F_i[v].$$
 (2.8)

The condition:

$$C[i][v] = 0 \ \forall 1 \le i \le M \tag{2.9}$$

is called a Constraint for v.

In particular each linear functional implies a constraint.

#### **Definition 2.5** (Linear subspace).

Let V be a linear function space and  $C[\cdot][\cdot] = 0$  a constraint on V. Then we call

$$V_C := \{ v \in V | C[i][v] = 0 \ \forall i \in \{1, ..., M\} \}$$
 (2.10)

a linear subspace of V with respect to C.

 $V_C$  is a vector space itself, since the constraint functionals C[i] are linear. Typically,  $V_C$  becomes the space of test functions in our later problem.

#### **Definition 2.6** (Affine subspace).

Let V be a function space,  $V_C$  a linear subspace and  $g \in V$ . Then we call

$$V_g := \{ v + g | v \in V_C \} \subset V$$
 (2.11)

an affine subspace with respect to g and  $V_C$ .

In general,  $V_g$  is only a subspace of V and not a linear subspace (in the sense, that  $V_G$  is not a vector space itself in general). It will be the space of solutions in our later problem.

#### Definition 2.7 (Operator).

Let V be a linear function space,  $V_C \subset V$  a linear subspace,  $V'_C$  its dual and  $V_g \subset V$  an affine subspace. Then we call

$$G: V_q \to V_C' \tag{2.12}$$

an operator on  $V_g$ . If

$$G(\alpha v + \beta w) = \alpha G(v) + \beta G(w)$$

holds for all  $\alpha, \beta \in \mathbb{R}$  and for all  $v, w \in V_g$  the operator G is called linear.

In the subsequent sections, we are dealing with the following problem.

# Problem 2.8 (Sample problem).

Let V be a linear space,  $V_C \subset V$  a linear subspace,  $F \in V'_C$  a functional and  $V_g \subset V$  an affine subspace. Find  $u \in V_g$ , such that

$$G(u)[v] = F[v]$$
 for all  $v \in V_C$ .

In general, the functional F on the right hand side of our problem is linear. The (differential) operator G can be either linear or nonlinear.

# 3 Examples

# 3.1 Elliptic PDE

Let  $\Omega \subset \mathbb{R}^d$  denote a polygonal bounded domain,  $\mathcal{T}_H = \{T_1, ..., T_N\}$  a corresponding regular triangulation,  $\mathcal{N}_H = \{x_1, ...., x_{\tilde{N}}\}$  the set of nodes and  $\{\Phi_1, ...., \Phi_{\tilde{N}}\}$  the associated Lagrange basis of order 1. The (discrete) linear space of solutions is given by

$$V := \left\{ v_H \in C^0(\Omega) \middle| (v_H)_{|T} \in \mathbb{P}^1(T) \quad \forall T \in \mathcal{T}_H \right\}$$

and the linear subspace of testfunctions by  $V_0 := V \cap H_0^1(\Omega)$ . Now, let us consider the following discrete problem.

#### Problem 3.1.

For  $g \in V$  find  $u \in V$  with u = g on  $\partial \Omega$  and

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \qquad \qquad \text{for all } v \in V_0.$$

(Note:  $V_0$  can not be replaced by V).

Putting this into the general framework above, we define the (linear) functional  $F:V_0\to\mathbb{R}$  by

$$F[v] := \int_{\Omega} fv \qquad \text{for } v \in \mathring{V}.$$

 $V_0$  is a constraint subspace with the constraint  $C[i][v] := v(x_i^b) = 0$  for any boundary node  $x_i^b$  (i.e.  $\mathcal{N}_H \cap \partial \Omega = \{x_1^b, ..., x_{\overline{N}}^b\}$ ). We can therefore identify

$$V_0 = \{ v \in V | C[i][v] = 0 \ \forall 1 \le i \le \bar{N} \} =: V_C.$$

The affine subspace  $V_{g_H}$  is given by

$$V_{g_H} := \left\{ v + g_H \middle| v \in V \text{ and } g_H := \sum_{i=1}^{\tilde{N}} g(x_i) \Phi_i \right\}$$

and the (differential) operator  $G: V_{g_H} \to V'_C$  by

$$G(u)[v] := \int_{\Omega} \nabla u \cdot \nabla v \, dx.$$

With these notations the original problem reads:

Find 
$$u \in V_{q_H}$$
 with  $G(u) = F$  on  $V_C$ .

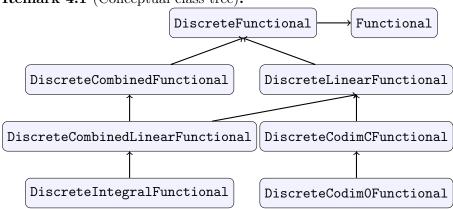
# 4 Realization in Dune-Fem-Functionals

In this section we describe the general programming concept. For a detailed description of these classes, see section? and the doxygen documentation. These classes are realized in a namespace Functionals in order to avoid conflicts with other existing Dune-Fem-classes. We do not distinguish between interfaces and realizations here, this is only intended as a conceptual overview.

#### 4.1 Functionals

The following diagram is intended to be a conceptual overview only. It is not intended to display a class hirarchy.

Remark 4.1 (Conceptual class tree).



The class Functional will not really be used. It is only there to provide us with the possibility to have all the following classes in a non-discrete way in the future. The only thing this class does is to enforce the  $\operatorname{operator}()$  for all functionals. The only method, the function v has to privide, is a method  $\operatorname{evaluate}(\operatorname{xGlobal})$ .

# Class 4.2 (Functional).

This class represents a functional F (see definition 2.2). It provides the base class for discrete and what-ever-else-there-will-be functionals.

#### Class definition:

class Functional< FunctionSpaceType >

# Methods:

RangeFieldType ret = operator( FunctionType function )		
description: This method represents the functional, applied to a function		
in:	FunctionType function $v$	
out:	RangeFieldType ret $F[v]$	

The class DiscreteFunctional is the actual base class for all functionals we use at the time being.

#### Class 4.3 (DiscreteFunctional).

This class represents a functional F (see definition 2.2), which can be applied to a discrete function.

#### Class definition:

class DiscreteFunctional< DiscreteFunctionSpaceType >

#### Methods:

RangeFieldTy	pe ret = operator( DiscreteFunctionType discreteFunct	ion )
description:	This method represents the functional, applied to a function.	
in:	FunctionType function $\ v$	
out:	RangeFieldType ret $F[v]$	

The DiscreteCombinedFunctional is more or less a pair of two DiscreteFunctionals. When its operator() is called, it just calles each operator() and adds the results.

### Class 4.4 (DiscreteCombinedFunctional).

Given two functionals  $F,G \in V'$ , this class represents the functional

$$F+G:V\to\mathbb{R}$$
 
$$v\mapsto F[v]+G[v].$$

This class is derived from DiscreteFunctional.

# Class definition:

class DiscreteCombinedFunctional < FirstFunctionalType, SecondFunctionalType >
: Functional

#### Methods:

<pre>RangeFieldType ret = operator( DiscreteFunctionType discreteFunction</pre>		
$description: \mid This \ method \ redefines \ {\tt DiscreteFunctional::operator()}.$		
in:	DiscreteFunctionType discreteFunction $v$	
out:	RangeFieldType ret $F[v] + G[v]$	

The DiscreteLinearFunctional is the base class for a wide range of interesting functionals – linear functionals. As stated in lemma 2.3, the most important property of linear functionals is, that its application to a discrete function can be split up and carried out by some kind of local application of the functionals to a local function.

#### Class 4.5 (DiscreteLinearFunctional).

This class represents a linear functional F (see definition 2.2). All linear functionals have to provide the method applyLocal() in addition to the method operator(). This class is derived from DiscreteFunctional.

#### Class definition:

class DiscreteLinearFunctional< DiscreteFunctionSpaceType >
: DiscreteFunctional

# Methods:

<pre>RangeFieldType ret = operator( DiscreteFunctionType discreteFunction )</pre>		
description:	description:   This method redefines DiscreteFunctional::operator().	
It makes use of the localization property of linear		
functionals (see lemma 2.3). It is implemented as a grid		
walk over all codim 0 entities which calls the method		
applyLocal() on each entity. Thus each linear functional		
	only has to implement the method applyLocal().	
in:	in: DiscreteFunctionType discreteFunction $v$	
out: RangeFieldType ret $F[v]$		
void applyLocal( LocalBasefunctionSetType localBasefunctionSet,		
LocalDoFVectorType returnVector )		
description: Given the localization property of a linear functional (see		

aescription:	Given the localization property of a linear functional (see	
	lemma 2.3), this method implements the vector $F[B_E]^E$	
in:	LocalBasefunctionSetType localBasefunctionSet $B_E$	
	LocalDoFVectorType returnVector	
out:	$F[B_E]^E := \left( F \left[ \varphi_{\mu_G(i)}^E \right] \right)_{i \in I_E}$	

# 4.2 Required classes

First of all we give an overview on the various classes that are required in our concept. In particular we comment on the functionality of each class.

# typedef Constraint < FunctionalType > ConstraintType;

- $\circ$  various realizations of constraints C are possible (boundary conditions, periodicity, zero-average, ...); they are derived from the general Constraint class
- $\circ$  mapping an element  $v \in V$  on an element  $v_C \in V_C$  is not unique, therefore 'applying a constraint' to a general function v means that we project v on  $V_C$  with respect to certain scalar product; in the discrete setting these projections are typically straight forward

- o required methods:
- · method: apply( numberOfConstraint, function )  $\leftrightarrow$  find  $v_C \in V_C$  which is 'close' to v and which fulfills  $C[i][v_C] = 0$ , i is the index of the functional (in our functional vector), v is an analytical function
- · method: apply( numberOfConstraint, discreteFunction )  $\leftrightarrow$  find  $v_C \in V_C$  which is 'close' to  $v_H$  and which fulfills  $C[i][v_C] = 0$ , i is the index of the functional (in our functional vector),  $v_H$  is a discrete function; typically we simply change the value of  $v_H$  in a certain number of nodes
- method: applyLocal( numberOfConstraint, localBasefunctionSet, localBasefunctionSet ) → again, an abstract method depending on the specific type of the constraint; it returns local contributions for a specific grid element; it is required for assembling the system matrix in our system of equations; details are given later
- method: applyLocal( localBasefunctionSet, localBasefunctionSet ) 

   ) use applyLocal( numberOfConstraint, localBasefunctionSet, localBasefunctionSet ) for all numberOfConstraint
- other methods depending on the specific type of a constraint (e.g. DirichletConstraint)?
- constraints are used to construct a 'constraint subspace' for the user, nothing else has to be done with the constraints

# typedef LinearSubspace < DiscreteFunctionSpace, ConstraintType > LinearSubspaceType;

- o derived from DiscreteFunctionSpace
- all the information about the constraint is in our subspace
- $\circ$  we can extract the constraint that it was constructed from
- o formally the subspace is of the same size as DiscreteFunctionSpace
- in particular an object of LinearSubspace becomes the space of test functions in our later problem

#### typedef AffineSubspace < LinearSubspace > AffineSubspaceType;

- the space of the solution
- $\circ$  initialized with a fixed discrete function  $v_H$ : 'AffineSubspace =  $v_H$  + LinearSubspace'
- o AffineSubspace-class derived from DiscreteFunctionSpace

```
typedef Operator< LinearSubspaceType, AffineSubspaceType,
    MatrixObjectTraits > DifferentialOperatorType;
```

- can be derived from the dune-fem Operator-class, later it should be implemented independently
- $\circ \ \ Operator: Affine Subspace \rightarrow (Linear Subspace)'$
- if required: automatically assembles the correct system matrix (which is a quadratic sparse row matrix) with respect to the subspaces (i.e. with respect to the constraints)
- simplified we can say: the *linear subspace* tells us which lines we must substitute in our later system of equations and the *affine subspace* tells us by what we must substitute these lines.
- usage of a DifferentialOperatorType-object identical to the old usage of an Operator-object
- o get system matrix with operator.systemMatrix();

Algebraic classes (assembling of system matrix and right hand side):

To assemble the right hand side in our system of equations: typedef FunctionalAssembler < FunctionalType, AffineSubspace > FunctionalAssemblerType;

To assemble the correct system matrix (with respect to the subspaces): typedef OperatorAssembler < OperatorType > OperatorAssemblerType;

• incorporates something like: assembleSystemMatrix(); constraints.apply( systemMatrix() );

Both classes might be incorporated in a general FunctionalSolverInterface, so that the user does not need to care about the system assemblers.

#### 4.3 Draft

Essential classes:

```
typedef Dune::SparseRowMatrixTraits < DiscreteFunctionSpace, DiscreteFunctionSpace
> MatrixObjectTraits;
typedef Operator< LinearSubspaceType, AffineSubspaceType,</pre>
   MatrixObjectTraits > DiffOperatorType;
// algebraic system assemblers:
typedef OperatorAssembler < OperatorType > OperatorAssemblerType;
typedef FunctionalAssembler < FunctionalType, AffineSubspace > FunctionalAssemblerType;
// CG scheme
typedef CGInverseOp< DiscreteFunctionType, OperatorAssembler > InverseOperatorType;
Main code:
DiscreteFunctionType rhs( "right hand side", discreteFunctionSpace );
// use a right hand side assembler class to apply 'functional+constraints' to right hand
side vector
FunctionalAssemblerType rhsAssembler ( functional, affineSubspace );
rhsAssembler.assemble( rhs );
// behaves like the old Operator-class of Dune-Fem:
OperatorAssemblerType systemMatrixAssembler ( differentialOperator );
// 'differentialOperator' contains correct 'systemMatrix()':
InverseOperatorType cg( systemMatrixAssembler, 1e-6, 1e-8 );
cg( rhs, solution );
We might think about hiding this main code behind a 'FunctionalSolver-
Interface', so that the user can simply call:
   cg( differentialOperator, functional, affineSubspace, solution );
(i.e. FunctionalSolverInterface < Operator, Functional, AffineSubspace >
Comparison with 'old' main code (for laplace operator and zero boundary
condition):
DiscreteFunctionType rhs( "rhs", discreteFunctionSpace );
AssembledFunctional < Functional Type > rhsFunctional ( disceretFunctionSpace, functional
);
rhsFunctional.assemble( rhs );
typedef LaplaceOperator< DiscreteFunctionType, MatrixObjectTraits > LaplaceOperatorType;
// apply constraints
bool hasDirBoundary = constraints.apply( laplaceOperator.systemMatrix(), rhs,
```

```
solution );
```

```
InverseOperatorType cg( laplaceOperator, 1e-6, 1e-8 );
cg( rhs, solution );
```

The essential difference is that the (differential) operator already knows the correct system matrix (due to the subspaces, that know the constraints). Therefore the user does not need some kind of 'constraints.apply' method (this happens internally in the two system assemblers).

# 5 Realization of Functionals

# 5.1 Integral Functionals

**Definition 5.1** (Integral functional).

Let V be a vector space,  $u \in V$  and  $f \in V^*$ . If f[u] can be decomposed as

$$f[u] = \sum_{c=0}^{dim} f^c[u],$$
 (5.1)

where  $f^c \in V^*$  are codim c integral functionals, which can be written as

$$f^{c}[u] = \int_{\omega^{c}} \tilde{f}^{c}[u] \tag{5.2}$$

for a set  $\omega^c$  of codimension c and a functional  $\tilde{f}^c \in V^*$ , then f is called an integral functional.

#### Lemma 5.2 (Localization property of integral functionals).

Let  $V_G$  be a discrete function space and  $f \in V_G^*$  an integral functional. Then it holds that

$$f[u] = \sum_{E \in G^0} \sum_{i \in I_E} u_i^E \sum_{c=0}^{dim} f^c[\varphi_i^E]$$

$$= \sum_{E \in G^0} u^E \cdot \left( \sum_{c=0}^{dim} \int_{G_E^0} \tilde{f}^c[B_E]^E \right), \tag{5.3}$$

where (...) is to be understood as the vector

$$\left(\sum_{c=0}^{\dim} \int_{G_{\mathcal{D}}^{0}} \tilde{f}^{c}[B_{E}]^{E}\right) := \left(\sum_{c=0}^{\dim} \int_{G_{\mathcal{D}}^{c}} \tilde{f}^{c}[\varphi_{i}^{E}]\right)_{i \in I_{E}}, \tag{5.4}$$

where  $G_E^c$  is "the set of all codim c entities, that lie inside E".

# Class 5.3 (LocalOperationProvider).

Represents the operation  $\tilde{f}^c[\varphi_i^E]$ , e.g.  $\tilde{f}^c[\varphi_i^E] = f(x)\varphi_i^E(x)$ . This class has to be provided by the user in order to define a CodimIntegralFunctional (see below).

number	Given a point x in local coordinates, returns $\tilde{f}^c[\varphi_i^E](x)$ ,
= apply( function,	where $\varphi_i^E$ is given as function and some function
localPoint,	associated with the functional can be given as
<pre>functionalFunction = 1 )</pre>	functionalFunction

Class 5.4 (CodimIntegralFunctional < LocalOperationProvider >: LinearFunctional). Represents a codim c functional  $f^c[u]$ . A CodimIntegralFunctional provides an additional method prepareLocalIntegration() to facilitate the integration in

IntegralFunctional::applyLocal() (see below). There should be derived classes for each codimension, which, together with a suitable LocalOperationProvider, can be given to an IntegralFunctional to provide something like an L2Functional for the user.

number	Inherited from LinearFunctional.
= operator( function )	
vector	Redefines LinearFunctional::applyLocal().
= applyLocal( localBasefunctionSet )	Given $B_E$ , computes $(f^c[\varphi_i^E])_{i \in I_E}$ by
	doing a codim c integration by quadrature
	$and \ calling \ {\tt prepareLocalIntegration}$
	for each quadrature point.
vector	Given $B_E$ and a point $x$ in local
= prepareLocalIntegration(	coordinates, returns $\tilde{f}^c[\varphi_i^E](x)$ by calling
localBasefunctionSet	$the \ underlying \ { t Local Operation Provider}.$
localPoint )	

Class 5.5 (IntegralFunctional < CodimIntegralFunctionals >: LinearFunctional). Represents an integral functional. This is like a CombinedLinearFunctional (see somewhere), but the integration in applyLocal() is only done once, calling

prepareLocalIntegration() on each CodimIntegralFunctional.

number	Inherited from LinearFunctional.
= operator( function )	
vector	Redefinition of
= applyLocal( localBasefunctionSet )	LinearFunctional::applyLocal().
	Given $B_E$ , computes $(f^c[\varphi_i^E])_{i \in I_E}$ by
	doing a codim c integration for each given
	codim by quadrature and calling
	prepareLocalIntegration() of each
	CodimIntegralFunctional for each
	quadrature point.

# 6 Realization of Constraints

Maybe, we should discuss the general concept first.

 $\label{thm:example:constraint} Example: \texttt{ConstraintType::DirichletConstraint dirConstraint(function)};$ 

# References

[1] A. Dedner, R. Klöfkorn, M. Nolte, and M. Ohlberger. A generic interface for parallel and adaptive discretization schemes: abstraction principles and the dune-fem module. *Computing*, 90(3-4):165–196, 2010.